



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2020 – 09:33 pm BST

PDB ID : 5H8I  
Title : Crystal structure of *Medicago truncatula* N-carbamoylputrescine amidohydrolase (MtCPA) in complex with N-(dihydroxymethyl)putrescine  
Authors : Sekula, B.; Ruszkowski, M.; Malinska, M.; Dauter, Z.  
Deposited on : 2015-12-23  
Resolution : 1.97 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

<https://www.wwpdb.org/validation/2017/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:

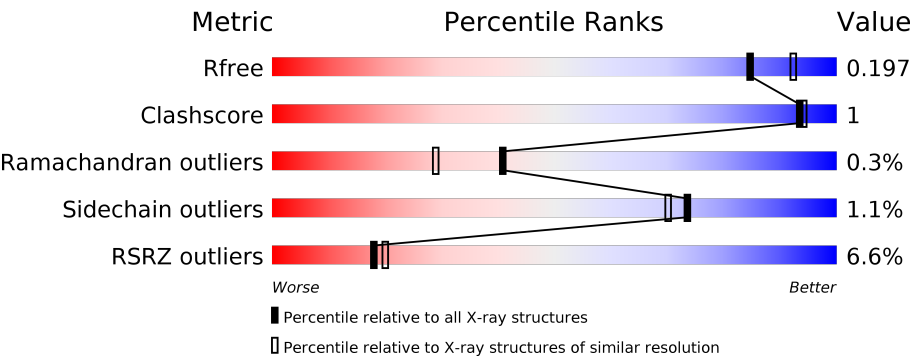
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 1.97 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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 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	304	<div><div>11%</div><div><div></div><div>92%</div><div>5%</div><div></div></div><div></div></div>
1	B	304	<div><div>4%</div><div><div></div><div>94%</div><div></div><div></div></div><div></div></div>
1	C	304	<div><div>3%</div><div><div></div><div>94%</div><div>5%</div><div></div></div><div></div></div>
1	D	304	<div><div>%</div><div><div></div><div>94%</div><div></div><div></div></div><div></div></div>
1	E	304	<div><div>%</div><div><div></div><div>96%</div><div></div><div></div></div><div></div></div>
1	F	304	<div><div>%</div><div><div></div><div>94%</div><div></div><div></div></div><div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	304	<div><div></div><div>8%</div><div>90%</div><div>7%</div><div></div><div></div></div>
1	H	304	<div><div></div><div>34%</div><div>86%</div><div>6%</div><div>7%</div><div></div></div>
1	I	304	<div><div></div><div>9%</div><div>93%</div><div></div><div></div><div></div></div>
1	J	304	<div><div></div><div>3%</div><div>94%</div><div></div><div></div><div></div></div>
1	K	304	<div><div></div><div>4%</div><div>96%</div><div></div><div></div><div></div></div>
1	L	304	<div><div></div><div>%</div><div>96%</div><div></div><div></div><div></div></div>
1	M	304	<div><div></div><div>%</div><div>95%</div><div></div><div></div><div></div></div>
1	N	304	<div><div></div><div>%</div><div>93%</div><div>5%</div><div></div></div>
1	O	304	<div><div></div><div>2%</div><div>95%</div><div></div><div></div><div></div></div>
1	P	304	<div><div></div><div>19%</div><div>88%</div><div>6%</div><div>5%</div><div></div></div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 42615 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 N-carbamoylputrescine amidohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	3	0
			2359	1509	405	435	10			
1	B	298	Total	C	N	O	S	0	2	0
			2373	1517	409	439	8			
1	C	301	Total	C	N	O	S	0	4	0
			2402	1536	412	444	10			
1	D	298	Total	C	N	O	S	0	5	0
			2384	1527	409	439	9			
1	E	297	Total	C	N	O	S	0	3	0
			2370	1516	408	438	8			
1	F	298	Total	C	N	O	S	0	4	0
			2381	1522	409	441	9			
1	G	295	Total	C	N	O	S	0	1	0
			2348	1501	405	434	8			
1	H	282	Total	C	N	O	S	0	2	0
			2253	1444	387	412	10			
1	I	293	Total	C	N	O	S	0	1	0
			2327	1487	401	430	9			
1	J	298	Total	C	N	O	S	0	4	0
			2380	1523	409	439	9			
1	K	301	Total	C	N	O	S	0	5	0
			2406	1540	412	444	10			
1	L	298	Total	C	N	O	S	0	4	0
			2380	1523	409	439	9			
1	M	297	Total	C	N	O	S	0	5	0
			2376	1523	408	436	9			
1	N	298	Total	C	N	O	S	0	4	0
			2381	1522	409	441	9			
1	O	297	Total	C	N	O	S	0	2	0
			2367	1513	408	438	8			
1	P	289	Total	C	N	O	S	0	2	0
			2304	1475	395	424	10			

There are 48 discrepancies between the modelled and reference sequences:

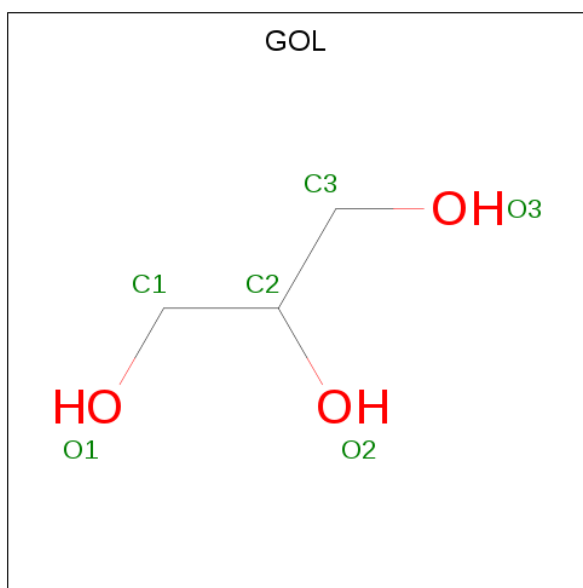
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP G7ITU5
A	-1	ASN	-	expression tag	UNP G7ITU5
A	0	ALA	-	expression tag	UNP G7ITU5
B	-2	SER	-	expression tag	UNP G7ITU5
B	-1	ASN	-	expression tag	UNP G7ITU5
B	0	ALA	-	expression tag	UNP G7ITU5
C	-2	SER	-	expression tag	UNP G7ITU5
C	-1	ASN	-	expression tag	UNP G7ITU5
C	0	ALA	-	expression tag	UNP G7ITU5
D	-2	SER	-	expression tag	UNP G7ITU5
D	-1	ASN	-	expression tag	UNP G7ITU5
D	0	ALA	-	expression tag	UNP G7ITU5
E	-2	SER	-	expression tag	UNP G7ITU5
E	-1	ASN	-	expression tag	UNP G7ITU5
E	0	ALA	-	expression tag	UNP G7ITU5
F	-2	SER	-	expression tag	UNP G7ITU5
F	-1	ASN	-	expression tag	UNP G7ITU5
F	0	ALA	-	expression tag	UNP G7ITU5
G	-2	SER	-	expression tag	UNP G7ITU5
G	-1	ASN	-	expression tag	UNP G7ITU5
G	0	ALA	-	expression tag	UNP G7ITU5
H	-2	SER	-	expression tag	UNP G7ITU5
H	-1	ASN	-	expression tag	UNP G7ITU5
H	0	ALA	-	expression tag	UNP G7ITU5
I	-2	SER	-	expression tag	UNP G7ITU5
I	-1	ASN	-	expression tag	UNP G7ITU5
I	0	ALA	-	expression tag	UNP G7ITU5
J	-2	SER	-	expression tag	UNP G7ITU5
J	-1	ASN	-	expression tag	UNP G7ITU5
J	0	ALA	-	expression tag	UNP G7ITU5
K	-2	SER	-	expression tag	UNP G7ITU5
K	-1	ASN	-	expression tag	UNP G7ITU5
K	0	ALA	-	expression tag	UNP G7ITU5
L	-2	SER	-	expression tag	UNP G7ITU5
L	-1	ASN	-	expression tag	UNP G7ITU5
L	0	ALA	-	expression tag	UNP G7ITU5
M	-2	SER	-	expression tag	UNP G7ITU5
M	-1	ASN	-	expression tag	UNP G7ITU5
M	0	ALA	-	expression tag	UNP G7ITU5
N	-2	SER	-	expression tag	UNP G7ITU5
N	-1	ASN	-	expression tag	UNP G7ITU5
N	0	ALA	-	expression tag	UNP G7ITU5

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Chain	Residue	Modelled	Actual	Comment	Reference
O	-2	SER	-	expression tag	UNP G7ITU5
O	-1	ASN	-	expression tag	UNP G7ITU5
O	0	ALA	-	expression tag	UNP G7ITU5
P	-2	SER	-	expression tag	UNP G7ITU5
P	-1	ASN	-	expression tag	UNP G7ITU5
P	0	ALA	-	expression tag	UNP G7ITU5

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		

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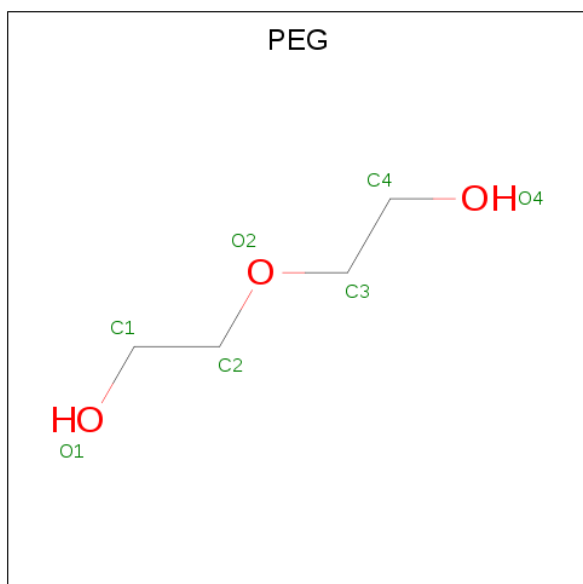
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	G	1	Total	C	O	0	0
			6	3	3		
2	H	1	Total	C	O	0	0
			6	3	3		
2	I	1	Total	C	O	0	0
			6	3	3		
2	I	1	Total	C	O	0	0
			6	3	3		
2	J	1	Total	C	O	0	0
			6	3	3		
2	J	1	Total	C	O	0	0
			6	3	3		
2	J	1	Total	C	O	0	0
			6	3	3		
2	J	1	Total	C	O	0	0
			6	3	3		
2	K	1	Total	C	O	0	0
			6	3	3		
2	K	1	Total	C	O	0	0
			6	3	3		
2	K	1	Total	C	O	0	0
			6	3	3		
2	L	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	M	1	Total	C	O	0	0
			6	3	3		
2	M	1	Total	C	O	0	0
			6	3	3		
2	N	1	Total	C	O	0	0
			6	3	3		
2	N	1	Total	C	O	0	0
			6	3	3		
2	N	1	Total	C	O	0	0
			6	3	3		
2	O	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	D	1	Total	C	O	0	0
			7	4	3		
3	D	1	Total	C	O	0	0
			7	4	3		
3	G	1	Total	C	O	0	0
			7	4	3		
3	J	1	Total	C	O	0	0
			7	4	3		

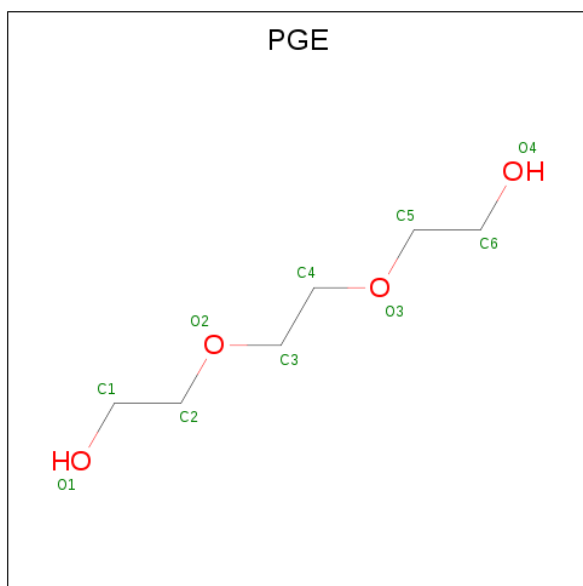
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	L	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



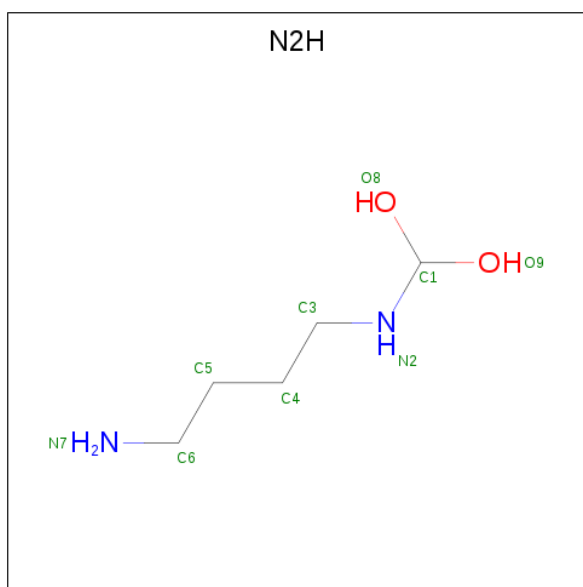
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		
4	C	1	Total	C	O	0	0
			10	6	4		
4	G	1	Total	C	O	0	0
			10	6	4		
4	J	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	K	1	Total	C	O	0	0
			4	2	2		
5	N	1	Total	C	O	0	0
			4	2	2		
5	P	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is (4-azanylbtylamino)methanediol (three-letter code: N2H) (formula: C<sub>5</sub>H<sub>14</sub>N<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			9	5	2	2		
6	C	1	Total	C	N	O	0	0
			9	5	2	2		
6	D	1	Total	C	N	O	0	0
			9	5	2	2		
6	E	1	Total	C	N	O	0	0
			9	5	2	2		
6	F	1	Total	C	N	O	0	0
			9	5	2	2		
6	G	1	Total	C	N	O	0	0
			9	5	2	2		
6	J	1	Total	C	N	O	0	0
			9	5	2	2		
6	K	1	Total	C	N	O	0	0
			9	5	2	2		
6	L	1	Total	C	N	O	0	0
			9	5	2	2		
6	M	1	Total	C	N	O	0	0
			9	5	2	2		
6	N	1	Total	C	N	O	0	0
			9	5	2	2		
6	O	1	Total	C	N	O	0	0
			9	5	2	2		

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	L	1	Total Na 1 1	0	0

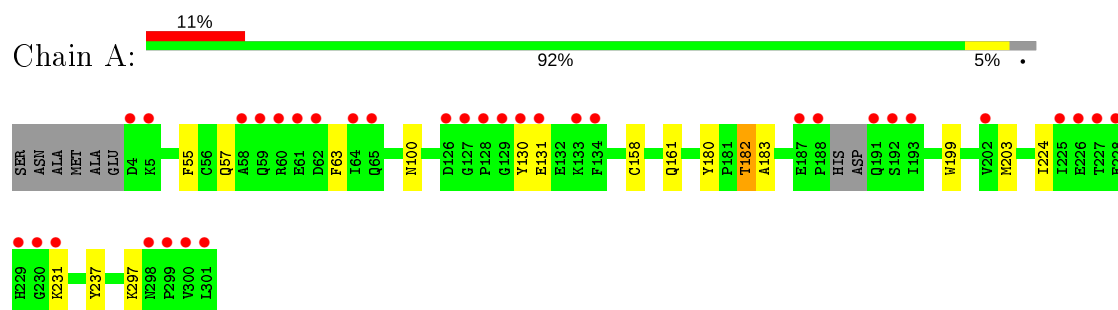
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	241	Total O 241 241	0	0
8	B	288	Total O 288 288	0	0
8	C	345	Total O 345 345	0	0
8	D	348	Total O 348 348	0	0
8	E	335	Total O 335 335	0	0
8	F	268	Total O 268 268	0	0
8	G	220	Total O 220 220	0	0
8	H	85	Total O 85 85	0	0
8	I	246	Total O 246 246	0	0
8	J	287	Total O 287 287	0	0
8	K	325	Total O 325 325	0	0
8	L	345	Total O 345 345	0	0
8	M	329	Total O 329 329	0	0
8	N	336	Total O 336 336	0	0
8	O	267	Total O 267 267	0	0
8	P	134	Total O 134 134	0	0

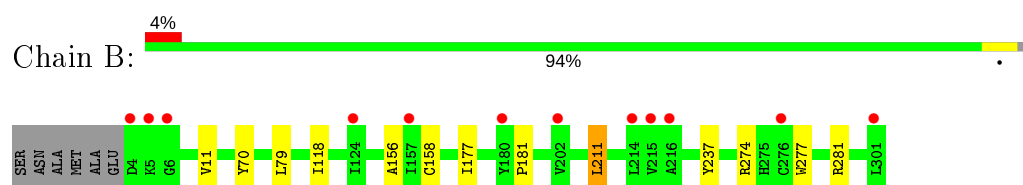
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

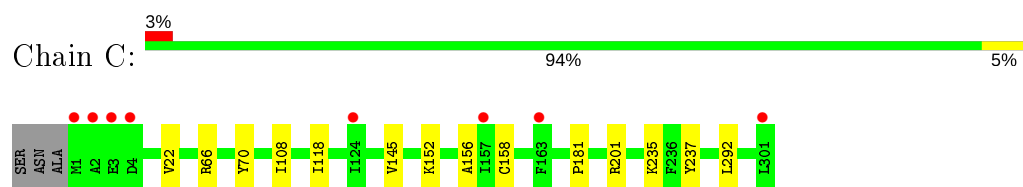
- Molecule 1: N-carbamoylputrescine amidohydrolase



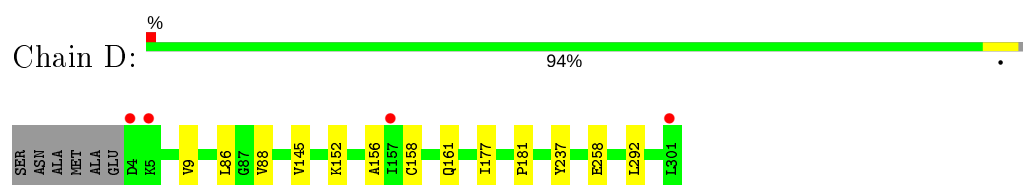
- Molecule 1: N-carbamoylputrescine amidohydrolase



- Molecule 1: N-carbamoylputrescine amidohydrolase



- Molecule 1: N-carbamoylputrescine amidohydrolase

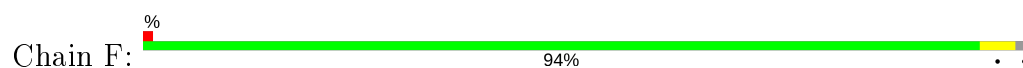


- Molecule 1: N-carbamoylputrescine amidohydrolase

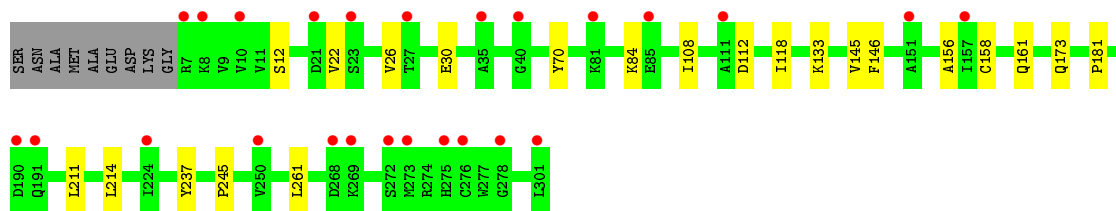
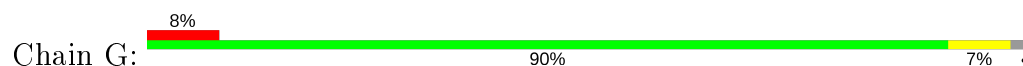




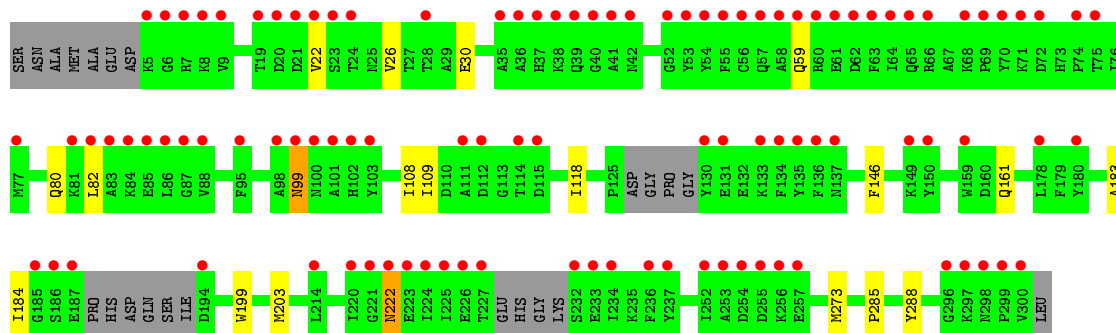
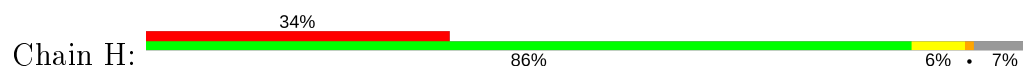
- Molecule 1: N-carbamoylputrescine amidohydrolase



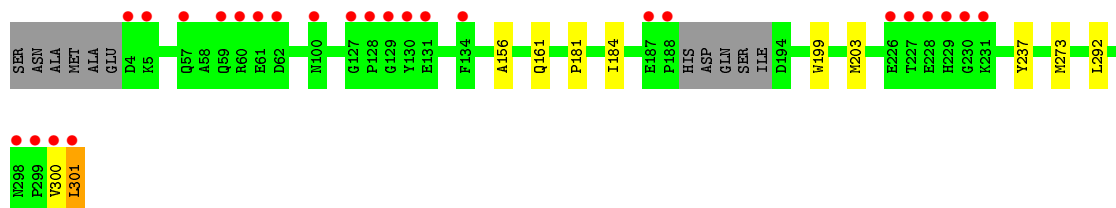
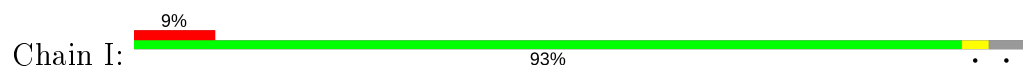
- Molecule 1: N-carbamoylputrescine amidohydrolase



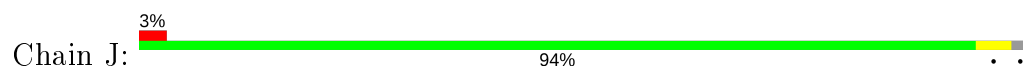
- Molecule 1: N-carbamoylputrescine amidohydrolase

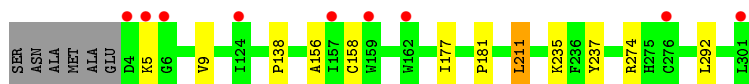


- Molecule 1: N-carbamoylputrescine amidohydrolase



- Molecule 1: N-carbamoylputrescine amidohydrolase





- Molecule 1: N-carbamoylputrescine amidohydrolase



- Molecule 1: N-carbamoylputrescine amidohydrolase



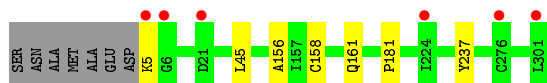
- Molecule 1: N-carbamoylputrescine amidohydrolase



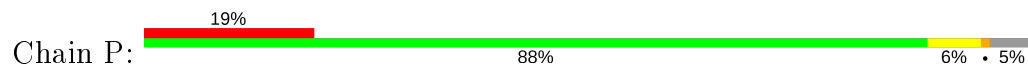
- Molecule 1: N-carbamoylputrescine amidohydrolase

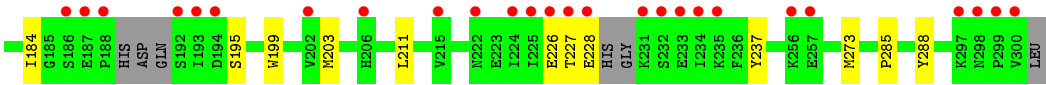


- Molecule 1: N-carbamoylputrescine amidohydrolase



- Molecule 1: N-carbamoylputrescine amidohydrolase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	152.13Å 211.06Å 208.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.55 – 1.97 39.55 – 1.97	Depositor EDS
% Data completeness (in resolution range)	98.5 (39.55-1.97) 98.5 (39.55-1.97)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.10 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.158 , 0.193 0.168 , 0.197	Depositor DCC
$R_{free}$ test set	2311 reflections (0.50%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.3	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 51.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	42615	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	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 42.83 % 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 1.9263e-04. 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, N2H, NA, EDO, PGE, PEG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.76	0/2422	0.72	0/3274
1	B	0.77	0/2435	0.71	0/3295
1	C	0.78	0/2470	0.75	0/3342
1	D	0.79	0/2455	0.73	0/3323
1	E	0.75	0/2435	0.72	0/3295
1	F	0.73	0/2449	0.73	0/3314
1	G	0.83	0/2407	0.68	0/3258
1	H	0.78	0/2308	0.68	0/3117
1	I	0.77	0/2384	0.71	0/3223
1	J	0.76	0/2448	0.72	0/3313
1	K	0.75	0/2477	0.72	0/3352
1	L	0.78	0/2448	0.72	0/3313
1	M	0.78	0/2447	0.72	0/3312
1	N	0.78	0/2449	0.71	0/3314
1	O	0.76	0/2429	0.68	0/3286
1	P	0.69	0/2360	0.67	0/3188
All	All	0.77	0/38823	0.71	0/52519

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2359	0	2334	13	0
1	B	2373	0	2340	6	0
1	C	2402	0	2377	8	0
1	D	2384	0	2363	6	0
1	E	2370	0	2340	1	0
1	F	2381	0	2349	6	0
1	G	2348	0	2311	12	0
1	H	2253	0	2231	12	0
1	I	2327	0	2292	6	0
1	J	2380	0	2354	6	0
1	K	2406	0	2386	5	0
1	L	2380	0	2354	3	0
1	M	2376	0	2359	3	0
1	N	2381	0	2349	7	0
1	O	2367	0	2333	2	0
1	P	2304	0	2277	11	0
2	A	18	0	24	0	0
2	B	12	0	16	0	0
2	C	24	0	32	2	0
2	D	12	0	16	0	0
2	E	24	0	32	0	0
2	F	12	0	16	0	0
2	G	6	0	8	0	0
2	H	6	0	8	2	0
2	I	12	0	16	0	0
2	J	24	0	32	1	0
2	K	18	0	24	0	0
2	L	6	0	8	0	0
2	M	12	0	16	0	0
2	N	18	0	24	0	0
2	O	6	0	8	1	0
3	A	7	0	10	0	0
3	D	14	0	20	1	0
3	G	7	0	10	0	0
3	J	7	0	10	0	0
3	L	7	0	10	0	0
4	A	10	0	14	0	0
4	C	10	0	14	0	0
4	G	10	0	14	0	0
4	J	10	0	14	0	0
5	A	4	0	6	0	0
5	C	4	0	6	0	0
5	D	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	K	4	0	6	0	0
5	N	4	0	6	0	0
5	P	4	0	6	0	0
6	B	9	0	0	0	0
6	C	9	0	0	0	0
6	D	9	0	0	0	0
6	E	9	0	0	0	0
6	F	9	0	0	0	0
6	G	9	0	0	0	0
6	J	9	0	0	0	0
6	K	9	0	0	0	0
6	L	9	0	0	0	0
6	M	9	0	0	0	0
6	N	9	0	0	0	0
6	O	9	0	0	0	0
7	L	1	0	0	0	0
8	A	241	0	0	2	0
8	B	288	0	0	0	0
8	C	345	0	0	2	0
8	D	348	0	0	0	0
8	E	335	0	0	0	0
8	F	268	0	0	2	0
8	G	220	0	0	1	0
8	H	85	0	0	1	0
8	I	246	0	0	1	0
8	J	287	0	0	1	0
8	K	325	0	0	1	0
8	L	345	0	0	1	0
8	M	329	0	0	1	0
8	N	336	0	0	2	0
8	O	267	0	0	0	0
8	P	134	0	0	0	0
All	All	42615	0	37781	104	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 1.

All (104) 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:N:228:GLU:HB3	8:N:688:HOH:O	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:145[B]:VAL:CG1	1:D:152:LYS:HG2	2.28	0.63
1:D:258:GLU:H	3:D:405:PEG:H21	1.63	0.63
1:P:99:ASN:HD22	1:P:100:ASN:H	1.47	0.63
1:D:86:LEU:HB2	1:D:88[B]:VAL:HG12	1.82	0.61
1:H:30:GLU:HG3	1:H:82:LEU:HD22	1.85	0.59
1:C:145[B]:VAL:CG1	1:C:152:LYS:HG2	2.32	0.58
1:M:273:MET:HE1	8:M:829:HOH:O	2.06	0.56
1:A:158:CYS:HA	1:A:182:THR:HG23	1.88	0.55
1:B:211:LEU:HD13	1:B:277:TRP:CE3	2.42	0.55
1:L:9[B]:VAL:HG11	1:L:177:ILE:HD11	1.90	0.54
1:P:98:ALA:O	1:P:99:ASN:ND2	2.40	0.54
1:N:22[A]:VAL:HG23	8:N:731:HOH:O	2.08	0.54
1:H:183:ALA:O	1:H:184:ILE:HD13	2.08	0.54
1:H:22:VAL:O	1:H:26:VAL:HG23	2.08	0.53
1:P:5:LYS:N	1:P:5:LYS:HD2	2.23	0.53
1:J:9[B]:VAL:HG11	1:J:177:ILE:HD11	1.89	0.53
1:A:161:GLN:HB2	1:A:203[B]:MET:HE3	1.90	0.52
1:H:199:TRP:O	1:H:203:MET:HG2	2.10	0.52
1:A:199:TRP:O	1:A:203[A]:MET:HG2	2.09	0.52
1:I:273:MET:HE1	8:I:746:HOH:O	2.08	0.52
1:I:199:TRP:O	1:I:203:MET:HG2	2.09	0.52
1:C:292:LEU:HD22	1:D:292:LEU:HD11	1.91	0.52
1:N:9[B]:VAL:HG11	1:N:177:ILE:HD11	1.91	0.52
1:F:70:TYR:CZ	1:F:118:ILE:HG23	2.46	0.51
1:G:108:ILE:HG13	1:G:146:PHE:CD2	2.46	0.51
1:G:84:LYS:HD3	1:G:112:ASP:O	2.11	0.51
1:H:273[A]:MET:HG3	2:H:401:GOL:O3	2.11	0.51
1:L:156:ALA:O	1:L:181:PRO:HD2	2.11	0.51
1:G:145[A]:VAL:HG21	1:G:173:GLN:O	2.11	0.51
1:P:199:TRP:O	1:P:203:MET:HG2	2.11	0.51
1:C:156:ALA:O	1:C:181:PRO:HD2	2.11	0.50
1:P:184:ILE:HD11	1:P:195:SER:OG	2.11	0.50
1:O:45:LEU:HD11	1:O:181:PRO:HG3	1.94	0.49
1:H:222:ASN:N	1:H:222:ASN:OD1	2.46	0.49
1:L:273:MET:HE1	8:L:843:HOH:O	2.12	0.48
1:K:145[B]:VAL:CG1	1:K:152:LYS:HG2	2.43	0.48
1:M:9[B]:VAL:HG11	1:M:177:ILE:HD11	1.95	0.48
1:J:138:PRO:HB2	2:J:405:GOL:H31	1.95	0.48
1:C:22[A]:VAL:HG23	8:C:691:HOH:O	2.13	0.48
1:P:59:GLN:NE2	1:P:131:GLU:HG2	2.28	0.48
1:G:12:SER:HA	1:G:261:LEU:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:273[A]:MET:CG	2:H:401:GOL:O3	2.62	0.48
1:J:156:ALA:O	1:J:181:PRO:HD2	2.14	0.47
1:D:9[A]:VAL:HG11	1:D:177:ILE:HD11	1.95	0.47
1:C:235:LYS:HE3	8:C:657:HOH:O	2.13	0.47
1:P:211:LEU:HD23	1:P:273[A]:MET:CE	2.45	0.47
1:F:4:ASP:N	8:F:503:HOH:O	2.46	0.47
1:K:22[A]:VAL:HG23	8:K:740:HOH:O	2.14	0.46
1:K:9[B]:VAL:HG11	1:K:177:ILE:HD11	1.97	0.46
1:A:57:GLN:OE1	1:A:57:GLN:HA	2.16	0.46
1:H:108:ILE:HG13	1:H:146:PHE:CD2	2.51	0.46
1:I:301:LEU:H	1:I:301:LEU:CD2	2.29	0.46
1:I:292:LEU:HD22	1:J:292:LEU:HD11	1.98	0.46
1:A:55:PHE:HB2	1:A:63:PHE:CD2	2.50	0.45
1:G:22:VAL:O	1:G:26:VAL:HG23	2.16	0.45
1:N:108:ILE:HG13	1:N:146:PHE:CD2	2.52	0.45
1:A:180:TYR:CD1	1:A:203[B]:MET:HE2	2.52	0.45
1:P:285:PRO:HA	1:P:288:TYR:CD2	2.52	0.45
1:A:161:GLN:OE1	1:A:182:THR:HG21	2.17	0.45
1:B:156:ALA:O	1:B:181:PRO:HD2	2.17	0.45
1:H:285:PRO:HA	1:H:288:TYR:CD2	2.52	0.45
1:O:156:ALA:O	1:O:181:PRO:HD2	2.16	0.45
1:A:161:GLN:HB2	1:A:203[A]:MET:SD	2.57	0.45
1:C:70:TYR:CZ	1:C:118:ILE:HG23	2.52	0.44
1:J:211:LEU:HD12	1:J:274:ARG:HA	2.00	0.44
1:P:227:THR:HG22	1:P:228:GLU:N	2.32	0.44
1:J:235:LYS:HE2	8:J:691:HOH:O	2.17	0.44
1:E:70:TYR:CZ	1:E:118:ILE:HG23	2.52	0.44
1:F:156:ALA:O	1:F:181:PRO:HD2	2.18	0.43
1:G:156:ALA:O	1:G:181:PRO:HD2	2.18	0.43
1:N:156:ALA:O	1:N:181:PRO:HD2	2.17	0.43
1:H:161:GLN:HB2	1:H:203:MET:SD	2.59	0.43
1:A:100:ASN:N	8:A:505:HOH:O	2.48	0.43
1:A:182:THR:HG22	1:A:183:ALA:H	1.83	0.43
1:C:201:ARG:HD3	2:C:405:GOL:H2	2.00	0.43
2:O:402:GOL:O1	1:P:273[A]:MET:HG3	2.18	0.43
1:G:211:LEU:HA	1:G:245:PRO:O	2.19	0.42
1:A:161:GLN:OE1	1:A:182:THR:CG2	2.68	0.42
1:D:156:ALA:O	1:D:181:PRO:HD2	2.19	0.42
1:H:273[A]:MET:HE1	8:H:585:HOH:O	2.19	0.42
1:P:161:GLN:HB2	1:P:203:MET:SD	2.59	0.42
1:F:133:LYS:HB3	1:G:133:LYS:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:4:ASP:N	1:F:269:LYS:HZ2	2.18	0.42
1:N:245:PRO:HB2	1:N:273:MET:HE3	2.01	0.42
1:M:108:ILE:HG13	1:M:146:PHE:CD1	2.55	0.41
1:N:22[B]:VAL:HG12	1:N:51:GLU:HB3	2.02	0.41
1:A:224:ILE:HG23	1:A:231:LYS:HG3	2.03	0.41
1:I:161:GLN:HB2	1:I:203:MET:SD	2.61	0.41
1:G:70:TYR:CZ	1:G:118:ILE:HG23	2.55	0.41
1:B:11:VAL:HG11	1:B:177:ILE:HD13	2.02	0.41
1:B:211:LEU:HD22	1:B:274:ARG:HA	2.02	0.41
1:G:214:LEU:HD23	1:G:214:LEU:C	2.41	0.41
1:A:203[B]:MET:HE1	8:A:502:HOH:O	2.20	0.41
1:F:22:VAL:HG23	8:F:702:HOH:O	2.20	0.41
1:G:22:VAL:HG23	8:G:573:HOH:O	2.20	0.41
1:I:156:ALA:O	1:I:181:PRO:HD2	2.21	0.41
1:K:45:LEU:HD11	1:K:181:PRO:HG3	2.02	0.41
1:B:79:LEU:HA	1:B:79:LEU:HD23	1.93	0.41
1:G:26:VAL:O	1:G:30:GLU:HG3	2.21	0.41
1:K:145[B]:VAL:CG1	1:K:152:LYS:CG	2.99	0.40
1:C:66:ARG:HB3	2:C:404:GOL:H2	2.03	0.40
1:B:70:TYR:CZ	1:B:118:ILE:HG23	2.57	0.40
1:H:80:GLN:HA	1:H:109:ILE:HG21	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	295/304 (97%)	282 (96%)	13 (4%)	0	100	100
1	B	298/304 (98%)	287 (96%)	10 (3%)	1 (0%)	41	29
1	C	303/304 (100%)	294 (97%)	8 (3%)	1 (0%)	41	29
1	D	301/304 (99%)	294 (98%)	6 (2%)	1 (0%)	41	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	298/304 (98%)	287 (96%)	10 (3%)	1 (0%)	41	29
1	F	300/304 (99%)	287 (96%)	12 (4%)	1 (0%)	41	29
1	G	294/304 (97%)	283 (96%)	10 (3%)	1 (0%)	41	29
1	H	276/304 (91%)	265 (96%)	9 (3%)	2 (1%)	22	11
1	I	290/304 (95%)	280 (97%)	10 (3%)	0	100	100
1	J	300/304 (99%)	292 (97%)	7 (2%)	1 (0%)	41	29
1	K	304/304 (100%)	293 (96%)	10 (3%)	1 (0%)	41	29
1	L	300/304 (99%)	289 (96%)	10 (3%)	1 (0%)	41	29
1	M	300/304 (99%)	292 (97%)	7 (2%)	1 (0%)	41	29
1	N	300/304 (99%)	289 (96%)	10 (3%)	1 (0%)	41	29
1	O	297/304 (98%)	288 (97%)	8 (3%)	1 (0%)	41	29
1	P	283/304 (93%)	277 (98%)	6 (2%)	0	100	100
All	All	4739/4864 (97%)	4579 (97%)	146 (3%)	14 (0%)	41	29

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	158	CYS
1	O	158	CYS
1	C	158	CYS
1	D	158	CYS
1	E	158	CYS
1	F	158	CYS
1	G	158	CYS
1	H	99	ASN
1	J	158	CYS
1	K	158	CYS
1	L	158	CYS
1	M	158	CYS
1	N	158	CYS
1	H	59	GLN

### 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	249/252 (99%)	244 (98%)	5 (2%)	55	48
1	B	250/252 (99%)	247 (99%)	3 (1%)	71	67
1	C	254/252 (101%)	252 (99%)	2 (1%)	81	80
1	D	253/252 (100%)	251 (99%)	2 (1%)	81	80
1	E	250/252 (99%)	248 (99%)	2 (1%)	81	80
1	F	252/252 (100%)	250 (99%)	2 (1%)	81	80
1	G	247/252 (98%)	245 (99%)	2 (1%)	81	80
1	H	237/252 (94%)	234 (99%)	3 (1%)	69	64
1	I	244/252 (97%)	240 (98%)	4 (2%)	62	56
1	J	252/252 (100%)	249 (99%)	3 (1%)	71	67
1	K	255/252 (101%)	253 (99%)	2 (1%)	81	80
1	L	252/252 (100%)	251 (100%)	1 (0%)	91	90
1	M	252/252 (100%)	250 (99%)	2 (1%)	81	80
1	N	252/252 (100%)	250 (99%)	2 (1%)	81	80
1	O	249/252 (99%)	246 (99%)	3 (1%)	71	67
1	P	243/252 (96%)	238 (98%)	5 (2%)	53	47
All	All	3991/4032 (99%)	3948 (99%)	43 (1%)	73	70

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	130	TYR
1	A	131	GLU
1	A	182	THR
1	A	237	TYR
1	A	297	LYS
1	B	211	LEU
1	B	237	TYR
1	B	281	ARG
1	C	108	ILE
1	C	237	TYR
1	D	161	GLN
1	D	237	TYR
1	E	161	GLN
1	E	237	TYR

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Mol	Chain	Res	Type
1	F	161	GLN
1	F	237	TYR
1	G	161	GLN
1	G	237	TYR
1	H	99	ASN
1	H	118	ILE
1	H	222	ASN
1	I	184	ILE
1	I	237	TYR
1	I	300	VAL
1	I	301	LEU
1	J	5	LYS
1	J	211	LEU
1	J	237	TYR
1	K	5	LYS
1	K	237	TYR
1	L	237	TYR
1	M	237	TYR
1	M	301	LEU
1	N	161	GLN
1	N	237	TYR
1	O	5	LYS
1	O	161	GLN
1	O	237	TYR
1	P	99	ASN
1	P	118	ILE
1	P	131	GLU
1	P	226	GLU
1	P	237	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	65	GLN
1	C	65	GLN
1	D	65	GLN
1	E	65	GLN
1	F	65	GLN
1	G	65	GLN
1	H	99	ASN
1	I	161	GLN
1	J	65	GLN

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Mol	Chain	Res	Type
1	J	173	GLN
1	K	65	GLN
1	L	65	GLN
1	M	65	GLN
1	N	65	GLN
1	O	65	GLN
1	P	59	GLN
1	P	99	ASN
1	P	161	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 64 ligands modelled in this entry, 1 is monoatomic - leaving 63 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	PEG	A	404	-	6,6,6	0.51	0	5,5,5	0.18	0
6	N2H	B	401	1	8,8,8	2.02	2 (25%)	5,8,8	1.74	1 (20%)
2	GOL	E	403	-	5,5,5	0.49	0	5,5,5	0.17	0
6	N2H	G	401	1	8,8,8	2.54	2 (25%)	5,8,8	1.62	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GOL	C	404	-	5,5,5	0.35	0	5,5,5	0.37	0
6	N2H	M	401	1	8,8,8	2.14	2 (25%)	5,8,8	2.37	1 (20%)
2	GOL	B	402	-	5,5,5	0.15	0	5,5,5	0.55	0
3	PEG	L	403	-	6,6,6	0.50	0	5,5,5	0.36	0
6	N2H	J	401	1	8,8,8	2.61	3 (37%)	5,8,8	1.77	1 (20%)
2	GOL	J	404	-	5,5,5	0.23	0	5,5,5	0.44	0
2	GOL	E	405	-	5,5,5	0.48	0	5,5,5	0.23	0
2	GOL	N	403	-	5,5,5	0.35	0	5,5,5	0.18	0
3	PEG	G	403	-	6,6,6	0.50	0	5,5,5	0.22	0
2	GOL	A	402	-	5,5,5	0.41	0	5,5,5	0.43	0
2	GOL	K	404	-	5,5,5	0.19	0	5,5,5	0.23	0
6	N2H	D	401	1	8,8,8	2.37	2 (25%)	5,8,8	2.19	2 (40%)
2	GOL	J	402	-	5,5,5	0.31	0	5,5,5	0.30	0
4	PGE	J	407	-	9,9,9	0.57	0	8,8,8	0.34	0
2	GOL	F	402	-	5,5,5	0.34	0	5,5,5	0.15	0
5	EDO	D	406	-	3,3,3	0.54	0	2,2,2	0.13	0
2	GOL	O	402	-	5,5,5	0.11	0	5,5,5	0.55	0
5	EDO	K	405	-	3,3,3	0.57	0	2,2,2	0.10	0
2	GOL	A	401	-	5,5,5	0.39	0	5,5,5	0.25	0
5	EDO	C	407	-	3,3,3	0.61	0	2,2,2	0.05	0
2	GOL	E	402	-	5,5,5	0.44	0	5,5,5	0.36	0
2	GOL	J	403	-	5,5,5	0.50	0	5,5,5	0.35	0
2	GOL	K	403	-	5,5,5	0.49	0	5,5,5	0.46	0
6	N2H	F	401	1	8,8,8	2.35	3 (37%)	5,8,8	1.59	1 (20%)
6	N2H	E	401	1	8,8,8	2.23	1 (12%)	5,8,8	2.28	1 (20%)
6	N2H	K	401	1	8,8,8	2.35	3 (37%)	5,8,8	2.18	1 (20%)
2	GOL	B	403	-	5,5,5	0.37	0	5,5,5	0.47	0
2	GOL	L	402	-	5,5,5	0.29	0	5,5,5	0.23	0
2	GOL	J	405	-	5,5,5	0.69	0	5,5,5	1.15	1 (20%)
2	GOL	H	401	-	5,5,5	0.38	0	5,5,5	0.77	0
2	GOL	D	402	-	5,5,5	0.39	0	5,5,5	1.13	0
2	GOL	I	401	-	5,5,5	0.43	0	5,5,5	0.25	0
3	PEG	J	406	-	6,6,6	0.51	0	5,5,5	0.27	0
2	GOL	M	402	-	5,5,5	0.27	0	5,5,5	0.52	0
6	N2H	L	401	1	8,8,8	2.16	2 (25%)	5,8,8	2.03	1 (20%)
2	GOL	C	405	-	5,5,5	0.33	0	5,5,5	0.42	0
5	EDO	A	406	-	3,3,3	0.52	0	2,2,2	0.29	0
6	N2H	C	401	1	8,8,8	2.08	2 (25%)	5,8,8	2.28	1 (20%)
2	GOL	G	402	-	5,5,5	0.37	0	5,5,5	0.26	0
5	EDO	N	405	-	3,3,3	0.47	0	2,2,2	0.26	0
6	N2H	O	401	1	8,8,8	2.39	1 (12%)	5,8,8	2.05	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GOL	D	403	-	5,5,5	0.39	0	5,5,5	0.41	0
2	GOL	N	402	-	5,5,5	0.44	0	5,5,5	0.65	0
3	PEG	D	404	-	6,6,6	0.48	0	5,5,5	0.36	0
2	GOL	C	403	-	5,5,5	0.25	0	5,5,5	0.35	0
5	EDO	P	401	-	3,3,3	0.58	0	2,2,2	0.16	0
2	GOL	A	403	-	5,5,5	0.33	0	5,5,5	0.30	0
4	PGE	C	406	-	9,9,9	0.54	0	8,8,8	0.25	0
2	GOL	E	404	-	5,5,5	0.31	0	5,5,5	0.38	0
6	N2H	N	401	1	8,8,8	2.33	2 (25%)	5,8,8	2.11	1 (20%)
2	GOL	K	402	-	5,5,5	0.26	0	5,5,5	0.61	0
2	GOL	I	402	-	5,5,5	0.66	0	5,5,5	0.61	0
2	GOL	N	404	-	5,5,5	0.41	0	5,5,5	0.43	0
2	GOL	C	402	-	5,5,5	0.65	0	5,5,5	0.43	0
4	PGE	G	404	-	9,9,9	0.48	0	8,8,8	0.26	0
2	GOL	M	403	-	5,5,5	0.39	0	5,5,5	0.15	0
3	PEG	D	405	-	6,6,6	0.47	0	5,5,5	0.65	0
2	GOL	F	403	-	5,5,5	0.60	0	5,5,5	0.82	0
4	PGE	A	405	-	9,9,9	0.54	0	8,8,8	0.47	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
3	PEG	A	404	-	-	2/4/4/4	-
6	N2H	B	401	1	-	0/4/6/6	-
2	GOL	E	403	-	-	2/4/4/4	-
6	N2H	G	401	1	-	0/4/6/6	-
2	GOL	C	404	-	-	0/4/4/4	-
6	N2H	M	401	1	-	0/4/6/6	-
2	GOL	B	402	-	-	4/4/4/4	-
3	PEG	L	403	-	-	2/4/4/4	-
6	N2H	J	401	1	-	0/4/6/6	-
2	GOL	J	404	-	-	2/4/4/4	-
2	GOL	E	405	-	-	0/4/4/4	-
2	GOL	N	403	-	-	0/4/4/4	-
3	PEG	G	403	-	-	1/4/4/4	-
2	GOL	A	402	-	-	0/4/4/4	-
2	GOL	K	404	-	-	0/4/4/4	-
6	N2H	D	401	1	-	0/4/6/6	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	J	402	-	-	4/4/4/4	-
4	PGE	J	407	-	-	4/7/7/7	-
2	GOL	F	402	-	-	2/4/4/4	-
5	EDO	D	406	-	-	1/1/1/1	-
2	GOL	O	402	-	-	2/4/4/4	-
5	EDO	K	405	-	-	1/1/1/1	-
2	GOL	A	401	-	-	0/4/4/4	-
5	EDO	C	407	-	-	1/1/1/1	-
2	GOL	E	402	-	-	4/4/4/4	-
2	GOL	J	403	-	-	4/4/4/4	-
2	GOL	K	403	-	-	4/4/4/4	-
6	N2H	F	401	1	-	0/4/6/6	-
6	N2H	E	401	1	-	0/4/6/6	-
6	N2H	K	401	1	-	0/4/6/6	-
2	GOL	B	403	-	-	1/4/4/4	-
2	GOL	L	402	-	-	0/4/4/4	-
2	GOL	J	405	-	-	2/4/4/4	-
2	GOL	H	401	-	-	0/4/4/4	-
2	GOL	D	402	-	-	1/4/4/4	-
2	GOL	I	401	-	-	0/4/4/4	-
3	PEG	J	406	-	-	3/4/4/4	-
2	GOL	M	402	-	-	3/4/4/4	-
6	N2H	L	401	1	-	1/4/6/6	-
2	GOL	C	405	-	-	2/4/4/4	-
5	EDO	A	406	-	-	1/1/1/1	-
6	N2H	C	401	1	-	0/4/6/6	-
2	GOL	G	402	-	-	2/4/4/4	-
5	EDO	N	405	-	-	1/1/1/1	-
6	N2H	O	401	1	-	0/4/6/6	-
2	GOL	D	403	-	-	0/4/4/4	-
2	GOL	N	402	-	-	4/4/4/4	-
3	PEG	D	404	-	-	2/4/4/4	-
2	GOL	C	403	-	-	0/4/4/4	-
5	EDO	P	401	-	-	1/1/1/1	-
2	GOL	A	403	-	-	1/4/4/4	-
4	PGE	C	406	-	-	4/7/7/7	-
2	GOL	E	404	-	-	0/4/4/4	-
6	N2H	N	401	1	-	0/4/6/6	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	K	402	-	-	2/4/4/4	-
2	GOL	I	402	-	-	2/4/4/4	-
2	GOL	N	404	-	-	0/4/4/4	-
2	GOL	C	402	-	-	3/4/4/4	-
4	PGE	G	404	-	-	1/7/7/7	-
2	GOL	M	403	-	-	4/4/4/4	-
3	PEG	D	405	-	-	3/4/4/4	-
2	GOL	F	403	-	-	2/4/4/4	-
4	PGE	A	405	-	-	4/7/7/7	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	O	401	N2H	C1-N2	5.96	1.57	1.41
6	D	401	N2H	C1-N2	5.82	1.57	1.41
6	G	401	N2H	C1-N2	5.75	1.57	1.41
6	N	401	N2H	C1-N2	5.75	1.57	1.41
6	K	401	N2H	C1-N2	5.65	1.56	1.41
6	E	401	N2H	C1-N2	5.64	1.56	1.41
6	J	401	N2H	C1-N2	5.46	1.56	1.41
6	F	401	N2H	C1-N2	5.33	1.56	1.41
6	L	401	N2H	C1-N2	5.06	1.55	1.41
6	M	401	N2H	C1-N2	5.05	1.55	1.41
6	C	401	N2H	C1-N2	5.00	1.55	1.41
6	B	401	N2H	C1-N2	4.62	1.54	1.41
6	G	401	N2H	C3-N2	3.17	1.53	1.47
6	J	401	N2H	O8-C1	3.09	1.48	1.40
6	J	401	N2H	C3-N2	3.06	1.53	1.47
6	M	401	N2H	O8-C1	2.60	1.46	1.40
6	B	401	N2H	O8-C1	2.54	1.46	1.40
6	F	401	N2H	C3-N2	2.52	1.52	1.47
6	K	401	N2H	C3-N2	2.47	1.52	1.47
6	C	401	N2H	C3-N2	2.41	1.52	1.47
6	L	401	N2H	O8-C1	2.34	1.46	1.40
6	D	401	N2H	O8-C1	2.23	1.45	1.40
6	F	401	N2H	O9-C1	2.14	1.45	1.40
6	N	401	N2H	C3-N2	2.09	1.51	1.47
6	K	401	N2H	O8-C1	2.02	1.45	1.40

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	401	N2H	O9-C1-O8	-5.06	100.85	111.32
6	E	401	N2H	O9-C1-O8	-4.78	101.43	111.32
6	C	401	N2H	O9-C1-O8	-4.65	101.70	111.32
6	D	401	N2H	O9-C1-O8	-4.41	102.21	111.32
6	N	401	N2H	O9-C1-O8	-4.36	102.29	111.32
6	K	401	N2H	O9-C1-O8	-4.36	102.30	111.32
6	O	401	N2H	O9-C1-O8	-4.35	102.32	111.32
6	L	401	N2H	O9-C1-O8	-4.11	102.82	111.32
6	J	401	N2H	O9-C1-O8	-3.59	103.89	111.32
6	B	401	N2H	O9-C1-O8	-3.49	104.11	111.32
6	F	401	N2H	O9-C1-O8	-3.20	104.71	111.32
6	G	401	N2H	O9-C1-O8	-3.17	104.76	111.32
2	J	405	GOL	O3-C3-C2	2.12	120.35	110.20
6	D	401	N2H	C4-C3-N2	-2.02	104.49	112.02

There are no chirality outliers.

All (90) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	403	GOL	C1-C2-C3-O3
2	J	404	GOL	O1-C1-C2-O2
2	J	402	GOL	C1-C2-C3-O3
2	O	402	GOL	C1-C2-C3-O3
2	J	403	GOL	C1-C2-C3-O3
2	K	403	GOL	C1-C2-C3-O3
2	J	405	GOL	C1-C2-C3-O3
2	M	402	GOL	O1-C1-C2-C3
2	C	405	GOL	O1-C1-C2-O2
2	G	402	GOL	O1-C1-C2-C3
2	K	402	GOL	O1-C1-C2-O2
2	K	402	GOL	O1-C1-C2-C3
2	I	402	GOL	C1-C2-C3-O3
2	I	402	GOL	O2-C2-C3-O3
2	C	402	GOL	C1-C2-C3-O3
2	C	402	GOL	O2-C2-C3-O3
2	M	403	GOL	C1-C2-C3-O3
2	F	403	GOL	C1-C2-C3-O3
4	J	407	PGE	O2-C3-C4-O3
4	C	406	PGE	O2-C3-C4-O3
2	E	402	GOL	O1-C1-C2-O2
2	K	403	GOL	O2-C2-C3-O3
2	J	405	GOL	O2-C2-C3-O3
3	A	404	PEG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	A	405	PGE	O1-C1-C2-O2
4	A	405	PGE	O3-C5-C6-O4
4	G	404	PGE	O1-C1-C2-O2
4	C	406	PGE	O1-C1-C2-O2
4	C	406	PGE	O3-C5-C6-O4
2	B	402	GOL	O1-C1-C2-C3
2	B	402	GOL	C1-C2-C3-O3
2	J	404	GOL	O1-C1-C2-C3
2	J	402	GOL	O1-C1-C2-C3
2	F	402	GOL	O1-C1-C2-C3
2	E	402	GOL	O1-C1-C2-C3
2	E	402	GOL	C1-C2-C3-O3
2	J	403	GOL	O1-C1-C2-C3
2	K	403	GOL	O1-C1-C2-C3
2	D	402	GOL	O1-C1-C2-C3
2	C	405	GOL	O1-C1-C2-C3
2	N	402	GOL	O1-C1-C2-C3
2	N	402	GOL	C1-C2-C3-O3
2	C	402	GOL	O1-C1-C2-C3
2	M	403	GOL	O1-C1-C2-C3
2	E	403	GOL	O2-C2-C3-O3
2	B	402	GOL	O1-C1-C2-O2
2	B	402	GOL	O2-C2-C3-O3
2	J	402	GOL	O2-C2-C3-O3
2	O	402	GOL	O2-C2-C3-O3
2	E	402	GOL	O2-C2-C3-O3
2	J	403	GOL	O1-C1-C2-O2
2	J	403	GOL	O2-C2-C3-O3
2	M	402	GOL	O1-C1-C2-O2
2	G	402	GOL	O1-C1-C2-O2
2	N	402	GOL	O1-C1-C2-O2
2	N	402	GOL	O2-C2-C3-O3
2	F	403	GOL	O2-C2-C3-O3
3	J	406	PEG	O1-C1-C2-O2
3	J	406	PEG	O2-C3-C4-O4
5	D	406	EDO	O1-C1-C2-O2
5	C	407	EDO	O1-C1-C2-O2
5	A	406	EDO	O1-C1-C2-O2
5	N	405	EDO	O1-C1-C2-O2
5	P	401	EDO	O1-C1-C2-O2
2	A	403	GOL	O1-C1-C2-C3
2	J	402	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	K	405	EDO	O1-C1-C2-O2
3	L	403	PEG	O2-C3-C4-O4
4	J	407	PGE	C1-C2-O2-C3
3	D	405	PEG	C4-C3-O2-C2
2	M	403	GOL	O2-C2-C3-O3
3	L	403	PEG	O1-C1-C2-O2
2	M	402	GOL	C1-C2-C3-O3
4	C	406	PGE	C1-C2-O2-C3
4	J	407	PGE	O1-C1-C2-O2
6	L	401	N2H	N2-C3-C4-C5
3	A	404	PEG	O2-C3-C4-O4
4	J	407	PGE	C3-C4-O3-C5
3	D	405	PEG	O2-C3-C4-O4
4	A	405	PGE	C4-C3-O2-C2
3	D	405	PEG	O1-C1-C2-O2
2	M	403	GOL	O1-C1-C2-O2
3	D	404	PEG	C4-C3-O2-C2
3	J	406	PEG	C4-C3-O2-C2
3	G	403	PEG	C4-C3-O2-C2
2	F	402	GOL	O1-C1-C2-O2
2	K	403	GOL	O1-C1-C2-O2
2	B	403	GOL	O2-C2-C3-O3
3	D	404	PEG	O1-C1-C2-O2
4	A	405	PGE	O2-C3-C4-O3

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	404	GOL	1	0
2	O	402	GOL	1	0
2	J	405	GOL	1	0
2	H	401	GOL	2	0
2	C	405	GOL	1	0
3	D	405	PEG	1	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	296/304 (97%)	0.33	34 (11%) 4 5	19, 32, 76, 95	0
1	B	298/304 (98%)	0.05	12 (4%) 38 40	17, 26, 43, 85	0
1	C	301/304 (99%)	-0.04	8 (2%) 54 56	16, 25, 38, 82	0
1	D	298/304 (98%)	-0.16	4 (1%) 77 78	16, 24, 36, 71	0
1	E	297/304 (97%)	-0.12	4 (1%) 77 78	17, 26, 38, 66	0
1	F	298/304 (98%)	-0.27	4 (1%) 77 78	17, 30, 43, 79	0
1	G	295/304 (97%)	0.54	25 (8%) 10 12	29, 42, 58, 70	0
1	H	282/304 (92%)	1.70	103 (36%) 0 0	32, 57, 91, 106	0
1	I	293/304 (96%)	0.21	26 (8%) 9 10	20, 30, 69, 113	0
1	J	298/304 (98%)	0.01	9 (3%) 50 52	17, 26, 41, 96	0
1	K	301/304 (99%)	0.00	12 (3%) 38 40	16, 28, 41, 86	0
1	L	298/304 (98%)	-0.18	2 (0%) 87 88	16, 24, 36, 76	0
1	M	297/304 (97%)	-0.12	4 (1%) 77 78	16, 24, 36, 59	0
1	N	298/304 (98%)	-0.29	3 (1%) 82 83	16, 25, 37, 69	0
1	O	297/304 (97%)	-0.05	6 (2%) 65 66	22, 35, 50, 78	0
1	P	289/304 (95%)	1.01	58 (20%) 1 0	23, 47, 87, 100	0
All	All	4736/4864 (97%)	0.16	314 (6%) 18 20	16, 29, 63, 113	0

All (314) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	300	VAL	8.5
1	I	301	LEU	8.4
1	I	230	GLY	8.1
1	P	192	SER	8.1
1	A	128	PRO	7.9

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Mol	Chain	Res	Type	RSRZ
1	I	229	HIS	7.8
1	A	193	ILE	7.8
1	A	301	LEU	7.8
1	H	58	ALA	7.3
1	P	4	ASP	7.3
1	H	134	PHE	7.3
1	P	58	ALA	6.9
1	P	134	PHE	6.8
1	H	100	ASN	6.6
1	H	135	TYR	6.2
1	P	100	ASN	6.2
1	I	128	PRO	6.2
1	P	227	THR	6.2
1	P	225	ILE	6.2
1	P	193	ILE	6.1
1	H	227	THR	5.8
1	A	4	ASP	5.8
1	P	99	ASN	5.8
1	H	21	ASP	5.7
1	F	4	ASP	5.7
1	C	2	ALA	5.7
1	J	4	ASP	5.6
1	H	187	GLU	5.6
1	A	229	HIS	5.5
1	P	63	PHE	5.5
1	A	188	PRO	5.5
1	K	2	ALA	5.5
1	H	256	LYS	5.5
1	H	59	GLN	5.5
1	J	5	LYS	5.5
1	I	228	GLU	5.4
1	A	192	SER	5.4
1	K	3	GLU	5.4
1	I	130	TYR	5.3
1	A	230	GLY	5.3
1	P	5	LYS	5.3
1	A	130	TYR	5.3
1	O	5	LYS	5.2
1	H	99	ASN	5.2
1	H	232	SER	5.1
1	H	186	SER	5.1
1	H	87	GLY	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	4	ASP	5.0
1	G	276	CYS	5.0
1	H	130	TYR	4.9
1	H	61	GLU	4.9
1	H	57	GLN	4.9
1	P	62	ASP	4.9
1	H	225	ILE	4.8
1	P	232	SER	4.8
1	H	102	HIS	4.8
1	A	227	THR	4.7
1	H	299	PRO	4.7
1	H	63	PHE	4.7
1	A	127	GLY	4.7
1	H	224	ILE	4.7
1	A	126	ASP	4.6
1	P	300	VAL	4.6
1	I	227	THR	4.6
1	H	221	GLY	4.5
1	A	228	GLU	4.5
1	H	62	ASP	4.5
1	B	5	LYS	4.5
1	H	77	MET	4.5
1	H	131	GLU	4.4
1	H	220	ILE	4.4
1	P	135	TYR	4.4
1	I	4	ASP	4.3
1	H	222	ASN	4.2
1	I	129	GLY	4.2
1	H	298	ASN	4.2
1	A	231	LYS	4.2
1	H	38	LYS	4.2
1	P	188	PRO	4.2
1	H	257	GLU	4.1
1	K	5	LYS	4.1
1	H	66	ARG	4.1
1	H	65	GLN	4.1
1	O	276	CYS	4.1
1	F	301	LEU	4.1
1	H	71	LYS	4.1
1	H	185	GLY	4.1
1	P	299	PRO	4.1
1	P	61	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
1	I	300	VAL	4.0
1	H	70	TYR	4.0
1	P	65	GLN	4.0
1	P	186	SER	4.0
1	H	111	ALA	4.0
1	P	60	ARG	4.0
1	A	131	GLU	4.0
1	H	133	LYS	3.9
1	O	301	LEU	3.9
1	H	194	ASP	3.9
1	H	86	LEU	3.9
1	I	299	PRO	3.8
1	H	253	ALA	3.8
1	P	298	ASN	3.8
1	G	191	GLN	3.8
1	H	255	ASP	3.7
1	O	6	GLY	3.7
1	H	35	ALA	3.7
1	H	20	ASP	3.7
1	I	231	LYS	3.7
1	H	226	GLU	3.6
1	P	194	ASP	3.6
1	A	61	GLU	3.6
1	H	137	ASN	3.6
1	P	224	ILE	3.6
1	P	228	GLU	3.6
1	E	5	LYS	3.6
1	H	74	PRO	3.6
1	H	101	ALA	3.6
1	I	298	ASN	3.6
1	P	187	GLU	3.6
1	N	4	ASP	3.6
1	H	98	ALA	3.5
1	H	233	GLU	3.5
1	G	269	LYS	3.5
1	H	297	LYS	3.5
1	C	1	MET	3.5
1	H	114	THR	3.5
1	C	3	GLU	3.5
1	K	4	ASP	3.4
1	B	6	GLY	3.4
1	A	299	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	H	81	LYS	3.4
1	A	300	VAL	3.4
1	H	24	THR	3.4
1	P	226	GLU	3.4
1	G	301	LEU	3.4
1	P	222	ASN	3.4
1	G	278	GLY	3.4
1	H	64	ILE	3.4
1	P	64	ILE	3.4
1	G	273	MET	3.4
1	L	4	ASP	3.4
1	D	4	ASP	3.3
1	I	187	GLU	3.3
1	H	82	LEU	3.3
1	N	5	LYS	3.3
1	P	178	LEU	3.3
1	B	301	LEU	3.2
1	P	59	GLN	3.2
1	I	188	PRO	3.2
1	G	272	SER	3.2
1	A	65	GLN	3.2
1	I	131	GLU	3.2
1	H	178	LEU	3.1
1	J	157	ILE	3.2
1	G	35	ALA	3.1
1	I	134	PHE	3.1
1	H	37	HIS	3.1
1	P	231	LYS	3.1
1	H	150	TYR	3.1
1	A	298	ASN	3.1
1	G	250	VAL	3.1
1	H	22	VAL	3.1
1	P	256	LYS	3.1
1	H	75	THR	3.1
1	G	81	LYS	3.1
1	M	5	LYS	3.1
1	H	54	TYR	3.1
1	I	127	GLY	3.1
1	H	252	ILE	3.0
1	C	4	ASP	3.0
1	O	21	ASP	3.0
1	H	60	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	H	103	TYR	3.0
1	I	100	ASN	3.0
1	H	39	GLN	3.0
1	H	72	ASP	3.0
1	P	180	TYR	3.0
1	P	98	ALA	3.0
1	H	254	ASP	3.0
1	H	234	ILE	2.9
1	K	1	MET	2.9
1	H	28	THR	2.9
1	P	130	TYR	2.9
1	P	233	GLU	2.9
1	P	21	ASP	2.9
1	F	5	LYS	2.9
1	K	124	ILE	2.9
1	G	111	ALA	2.9
1	G	268	ASP	2.9
1	A	5	LYS	2.9
1	A	129	GLY	2.8
1	H	84	LYS	2.8
1	P	297	LYS	2.8
1	A	59	GLN	2.8
1	A	191	GLN	2.8
1	C	301	LEU	2.8
1	H	19	THR	2.8
1	I	61	GLU	2.8
1	A	134	PHE	2.8
1	H	136	PHE	2.8
1	H	223	GLU	2.8
1	P	234	ILE	2.8
1	M	178	LEU	2.8
1	J	6	GLY	2.8
1	H	5	LYS	2.8
1	I	62	ASP	2.8
1	A	187	GLU	2.7
1	A	58	ALA	2.7
1	G	151	ALA	2.7
1	H	112	ASP	2.7
1	G	27	THR	2.7
1	H	41	ALA	2.7
1	G	85	GLU	2.7
1	N	301	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	64	ILE	2.7
1	B	157	ILE	2.7
1	H	6	GLY	2.7
1	C	157	ILE	2.7
1	E	178	LEU	2.7
1	A	62	ASP	2.6
1	H	83	ALA	2.6
1	H	40	GLY	2.6
1	P	215	VAL	2.6
1	I	226	GLU	2.6
1	H	69	PRO	2.6
1	A	226	GLU	2.6
1	H	52	GLY	2.6
1	H	159	TRP	2.6
1	K	157	ILE	2.6
1	G	23	SER	2.6
1	H	237	TYR	2.6
1	G	21	ASP	2.6
1	H	296	GLY	2.6
1	P	126	ASP	2.6
1	G	224	ILE	2.5
1	J	124	ILE	2.5
1	B	216	ALA	2.5
1	H	55	PHE	2.5
1	H	95	PHE	2.5
1	H	8	LYS	2.5
1	P	18	CYS	2.5
1	G	275	HIS	2.4
1	H	68	LYS	2.4
1	J	276[A]	CYS	2.4
1	G	7	ARG	2.4
1	B	202	VAL	2.4
1	H	236	PHE	2.4
1	G	8	LYS	2.4
1	B	124	ILE	2.4
1	P	69	PRO	2.4
1	E	301	LEU	2.4
1	K	191	GLN	2.4
1	D	157	ILE	2.4
1	A	202	VAL	2.4
1	J	301	LEU	2.4
1	B	180	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	K	163	PHE	2.4
1	D	5	LYS	2.4
1	K	301	LEU	2.3
1	P	156	ALA	2.3
1	F	191	GLN	2.3
1	P	82	LEU	2.3
1	H	23	SER	2.3
1	A	225	ILE	2.3
1	P	57	GLN	2.3
1	P	56	CYS	2.3
1	M	191	GLN	2.3
1	B	215	VAL	2.3
1	G	190	ASP	2.3
1	H	214	LEU	2.3
1	B	276	CYS	2.3
1	I	5	LYS	2.3
1	G	10	VAL	2.2
1	H	36	ALA	2.2
1	H	42	ASN	2.2
1	G	157	ILE	2.2
1	C	163	PHE	2.2
1	P	95	PHE	2.2
1	H	9	VAL	2.2
1	P	6	GLY	2.2
1	D	301	LEU	2.2
1	H	85	GLU	2.2
1	P	111	ALA	2.2
1	M	180	TYR	2.2
1	P	235	LYS	2.2
1	P	206	HIS	2.2
1	L	157	ILE	2.2
1	J	159	TRP	2.2
1	K	159	TRP	2.2
1	H	115	ASP	2.2
1	H	88	VAL	2.2
1	I	57	GLN	2.2
1	I	59	GLN	2.2
1	C	124	ILE	2.1
1	P	101	ALA	2.1
1	K	180	TYR	2.1
1	E	180	TYR	2.1
1	H	7	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	53	TYR	2.1
1	H	180	TYR	2.1
1	P	133	LYS	2.1
1	P	202	VAL	2.1
1	O	224	ILE	2.1
1	B	214	LEU	2.1
1	H	56	CYS	2.1
1	H	149	LYS	2.1
1	A	60	ARG	2.0
1	J	162	TRP	2.0
1	A	133	LYS	2.0
1	G	40	GLY	2.0
1	P	257	GLU	2.0
1	P	114	THR	2.0
1	I	60	ARG	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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
3	PEG	G	403	7/7	0.72	0.25	66,70,73,74	0
3	PEG	D	405	7/7	0.73	0.39	63,63,70,71	0
2	GOL	E	405	6/6	0.75	0.33	59,64,66,66	0
4	PGE	G	404	10/10	0.76	0.28	64,88,100,103	0
4	PGE	A	405	10/10	0.77	0.19	46,61,66,68	0
3	PEG	J	406	7/7	0.78	0.27	68,70,72,72	0
2	GOL	A	402	6/6	0.78	0.29	56,59,61,61	0
4	PGE	J	407	10/10	0.79	0.30	50,68,73,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	EDO	N	405	4/4	0.83	0.23	52,53,54,54	0
2	GOL	B	403	6/6	0.83	0.18	46,56,58,59	0
5	EDO	K	405	4/4	0.84	0.20	44,50,51,56	0
2	GOL	I	402	6/6	0.84	0.19	36,44,45,46	0
3	PEG	A	404	7/7	0.84	0.27	68,69,71,71	0
2	GOL	J	404	6/6	0.84	0.20	53,59,61,61	0
2	GOL	N	404	6/6	0.85	0.34	55,56,59,60	0
2	GOL	C	405	6/6	0.85	0.36	37,50,54,54	0
2	GOL	J	403	6/6	0.85	0.21	43,49,51,52	0
5	EDO	C	407	4/4	0.86	0.22	44,47,48,50	0
2	GOL	A	403	6/6	0.86	0.15	59,64,67,68	0
2	GOL	A	401	6/6	0.87	0.18	50,54,59,60	0
6	N2H	N	401	9/9	0.88	0.20	33,35,38,42	0
6	N2H	O	401	9/9	0.88	0.19	41,43,45,51	0
3	PEG	D	404	7/7	0.88	0.29	58,60,61,61	0
3	PEG	L	403	7/7	0.88	0.33	56,57,62,62	0
2	GOL	F	403	6/6	0.88	0.17	36,46,48,48	0
4	PGE	C	406	10/10	0.88	0.26	59,61,64,68	0
5	EDO	D	406	4/4	0.89	0.25	53,54,55,55	0
7	NA	L	404	1/1	0.89	0.24	52,52,52,52	0
2	GOL	E	403	6/6	0.89	0.19	49,58,64,71	0
2	GOL	C	404	6/6	0.89	0.17	48,56,59,60	0
6	N2H	F	401	9/9	0.90	0.16	39,40,41,45	0
5	EDO	P	401	4/4	0.90	0.17	49,51,52,54	0
5	EDO	A	406	4/4	0.90	0.22	50,50,51,52	0
2	GOL	J	402	6/6	0.90	0.17	38,44,47,53	0
6	N2H	M	401	9/9	0.90	0.20	24,27,35,37	0
2	GOL	I	401	6/6	0.91	0.18	44,45,48,50	0
2	GOL	D	403	6/6	0.91	0.20	34,40,45,50	0
6	N2H	B	401	9/9	0.91	0.20	30,33,37,37	0
6	N2H	G	401	9/9	0.91	0.16	44,45,45,46	0
6	N2H	K	401	9/9	0.91	0.20	31,32,39,41	0
2	GOL	J	405	6/6	0.91	0.23	29,33,38,39	6
2	GOL	K	402	6/6	0.92	0.18	41,47,51,56	0
2	GOL	H	401	6/6	0.92	0.14	57,61,62,63	0
6	N2H	E	401	9/9	0.92	0.18	31,32,36,38	0
2	GOL	E	402	6/6	0.92	0.13	40,50,54,58	0
2	GOL	B	402	6/6	0.92	0.14	39,45,47,52	0
2	GOL	N	402	6/6	0.92	0.13	39,49,52,56	0
2	GOL	F	402	6/6	0.93	0.26	41,47,52,53	0
6	N2H	L	401	9/9	0.93	0.18	28,32,36,38	0
2	GOL	K	403	6/6	0.93	0.14	37,45,49,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GOL	O	402	6/6	0.93	0.12	47,49,50,53	0
6	N2H	C	401	9/9	0.93	0.19	28,30,36,38	0
2	GOL	G	402	6/6	0.93	0.12	43,47,50,50	0
6	N2H	J	401	9/9	0.93	0.20	29,33,35,36	0
2	GOL	C	402	6/6	0.94	0.13	38,44,48,53	0
2	GOL	N	403	6/6	0.94	0.21	36,44,44,45	0
2	GOL	C	403	6/6	0.94	0.23	35,44,48,53	0
6	N2H	D	401	9/9	0.94	0.18	29,31,35,35	0
2	GOL	D	402	6/6	0.95	0.13	35,44,48,52	0
2	GOL	E	404	6/6	0.95	0.21	34,41,42,45	0
2	GOL	K	404	6/6	0.96	0.24	41,46,50,54	0
2	GOL	M	402	6/6	0.96	0.09	36,45,48,53	0
2	GOL	M	403	6/6	0.96	0.20	33,41,47,51	0
2	GOL	L	402	6/6	0.97	0.18	33,41,48,56	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.