



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 13, 2016 – 12:08 PM EDT

PDB ID : 5H8K
Title : Crystal structure of Medicago truncatula N-carbamoylputrescine amidohydrolase (MtCPA) C158S mutant
Authors : Sekula, B.; Ruszkowski, M.; Malinska, M.; Dauter, Z.
Deposited on : 2015-12-23
Resolution : 2.39 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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 : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027107

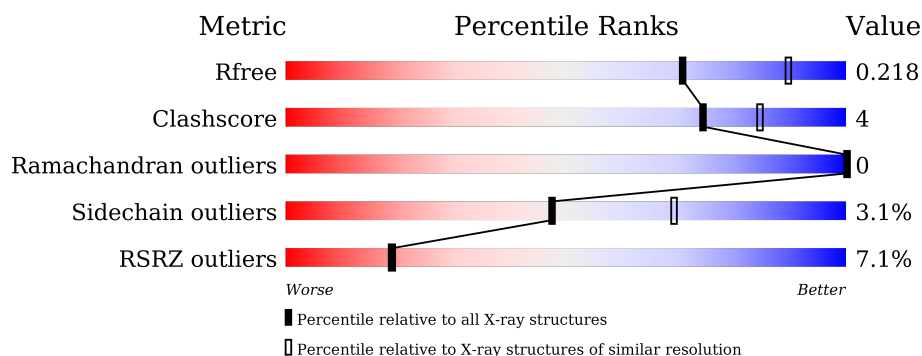
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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 ≥ 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	304	<div> <div>6%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>..</div> </div> </div>
1	B	304	<div> <div></div> <div>92%</div> <div>6%</div> <div>.</div> </div>
1	C	304	<div> <div></div> <div>91%</div> <div>8%</div> <div>..</div> </div>
1	D	304	<div> <div></div> <div>90%</div> <div>8%</div> <div>.</div> </div>
1	E	304	<div> <div>3%</div> <div> <div></div> <div>91%</div> <div>6%</div> <div>.</div> </div> </div>
1	F	304	<div> <div>4%</div> <div> <div></div> <div>89%</div> <div>8%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	304	
1	H	304	
1	I	304	
1	J	304	
1	K	304	
1	L	304	
1	M	304	
1	N	304	
1	O	304	
1	P	304	

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	GOL	A	401	-	-	-	X
2	GOL	B	401	-	-	-	X
2	GOL	B	404	-	-	-	X
2	GOL	C	401	-	-	-	X
2	GOL	C	402	-	-	-	X
2	GOL	C	403	-	-	-	X
2	GOL	D	402	-	-	-	X
2	GOL	D	403	-	-	-	X
2	GOL	D	404	-	-	-	X
2	GOL	E	401	-	-	-	X
2	GOL	E	403	-	-	-	X
2	GOL	E	404	-	-	-	X
2	GOL	F	401	-	-	-	X
2	GOL	F	403	-	-	-	X
2	GOL	G	401	-	-	-	X
2	GOL	G	402	-	-	-	X
2	GOL	G	403	-	-	-	X
2	GOL	J	401	-	-	-	X
2	GOL	J	402	-	-	-	X
2	GOL	K	403	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	L	401	-	-	-	X
2	GOL	L	402	-	-	-	X
2	GOL	L	403	-	-	-	X
2	GOL	M	401	-	-	-	X
2	GOL	M	403	-	-	-	X
2	GOL	N	401	-	-	-	X
2	GOL	N	403	-	-	-	X
2	GOL	N	404	-	-	-	X
2	GOL	O	401	-	-	-	X
3	EDO	A	403	-	-	-	X
3	EDO	C	405	-	-	-	X
3	EDO	D	405	-	-	-	X
3	EDO	I	403	-	-	-	X
3	EDO	K	404	-	-	-	X
4	PEG	L	404	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 40889 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	294	Total	C	N	O	S	0	1	0
			2333	1492	402	431	8			
1	B	297	Total	C	N	O	S	0	1	0
			2363	1509	408	439	7			
1	C	301	Total	C	N	O	S	0	1	0
			2390	1524	412	445	9			
1	D	298	Total	C	N	O	S	0	1	0
			2368	1511	409	440	8			
1	E	297	Total	C	N	O	S	0	0	0
			2357	1505	408	437	7			
1	F	298	Total	C	N	O	S	0	1	0
			2368	1511	409	440	8			
1	G	295	Total	C	N	O	S	0	0	0
			2344	1497	405	435	7			
1	H	278	Total	C	N	O	S	0	1	0
			2217	1423	383	403	8			
1	I	293	Total	C	N	O	S	0	1	0
			2327	1487	401	431	8			
1	J	298	Total	C	N	O	S	0	1	0
			2368	1511	409	440	8			
1	K	301	Total	C	N	O	S	0	2	0
			2396	1528	412	447	9			
1	L	298	Total	C	N	O	S	0	1	0
			2368	1511	409	440	8			
1	M	297	Total	C	N	O	S	0	1	0
			2360	1507	408	437	8			
1	N	298	Total	C	N	O	S	0	0	0
			2365	1509	409	440	7			
1	O	297	Total	C	N	O	S	0	0	0
			2357	1505	408	437	7			
1	P	288	Total	C	N	O	S	0	0	0
			2289	1465	394	423	7			

There are 64 discrepancies between the modelled and reference sequences:

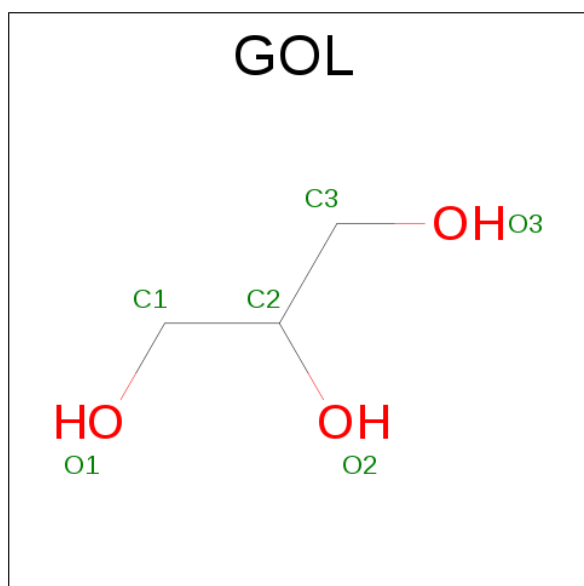
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A	-1	ASN	-	expression tag	UNP G7ITU5
A	0	ALA	-	expression tag	UNP G7ITU5
A	158	SER	CYS	engineered mutation	UNP G7ITU5
B	-2	SER	-	expression tag	UNP G7ITU5
B	-1	ASN	-	expression tag	UNP G7ITU5
B	0	ALA	-	expression tag	UNP G7ITU5
B	158	SER	CYS	engineered mutation	UNP G7ITU5
C	-2	SER	-	expression tag	UNP G7ITU5
C	-1	ASN	-	expression tag	UNP G7ITU5
C	0	ALA	-	expression tag	UNP G7ITU5
C	158	SER	CYS	engineered mutation	UNP G7ITU5
D	-2	SER	-	expression tag	UNP G7ITU5
D	-1	ASN	-	expression tag	UNP G7ITU5
D	0	ALA	-	expression tag	UNP G7ITU5
D	158	SER	CYS	engineered mutation	UNP G7ITU5
E	-2	SER	-	expression tag	UNP G7ITU5
E	-1	ASN	-	expression tag	UNP G7ITU5
E	0	ALA	-	expression tag	UNP G7ITU5
E	158	SER	CYS	engineered mutation	UNP G7ITU5
F	-2	SER	-	expression tag	UNP G7ITU5
F	-1	ASN	-	expression tag	UNP G7ITU5
F	0	ALA	-	expression tag	UNP G7ITU5
F	158	SER	CYS	engineered mutation	UNP G7ITU5
G	-2	SER	-	expression tag	UNP G7ITU5
G	-1	ASN	-	expression tag	UNP G7ITU5
G	0	ALA	-	expression tag	UNP G7ITU5
G	158	SER	CYS	engineered mutation	UNP G7ITU5
H	-2	SER	-	expression tag	UNP G7ITU5
H	-1	ASN	-	expression tag	UNP G7ITU5
H	0	ALA	-	expression tag	UNP G7ITU5
H	158	SER	CYS	engineered mutation	UNP G7ITU5
I	-2	SER	-	expression tag	UNP G7ITU5
I	-1	ASN	-	expression tag	UNP G7ITU5
I	0	ALA	-	expression tag	UNP G7ITU5
I	158	SER	CYS	engineered mutation	UNP G7ITU5
J	-2	SER	-	expression tag	UNP G7ITU5
J	-1	ASN	-	expression tag	UNP G7ITU5
J	0	ALA	-	expression tag	UNP G7ITU5
J	158	SER	CYS	engineered mutation	UNP G7ITU5
K	-2	SER	-	expression tag	UNP G7ITU5
K	-1	ASN	-	expression tag	UNP G7ITU5

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Chain	Residue	Modelled	Actual	Comment	Reference
K	0	ALA	-	expression tag	UNP G7ITU5
K	158	SER	CYS	engineered mutation	UNP G7ITU5
L	-2	SER	-	expression tag	UNP G7ITU5
L	-1	ASN	-	expression tag	UNP G7ITU5
L	0	ALA	-	expression tag	UNP G7ITU5
L	158	SER	CYS	engineered mutation	UNP G7ITU5
M	-2	SER	-	expression tag	UNP G7ITU5
M	-1	ASN	-	expression tag	UNP G7ITU5
M	0	ALA	-	expression tag	UNP G7ITU5
M	158	SER	CYS	engineered mutation	UNP G7ITU5
N	-2	SER	-	expression tag	UNP G7ITU5
N	-1	ASN	-	expression tag	UNP G7ITU5
N	0	ALA	-	expression tag	UNP G7ITU5
N	158	SER	CYS	engineered mutation	UNP G7ITU5
O	-2	SER	-	expression tag	UNP G7ITU5
O	-1	ASN	-	expression tag	UNP G7ITU5
O	0	ALA	-	expression tag	UNP G7ITU5
O	158	SER	CYS	engineered mutation	UNP G7ITU5
P	-2	SER	-	expression tag	UNP G7ITU5
P	-1	ASN	-	expression tag	UNP G7ITU5
P	0	ALA	-	expression tag	UNP G7ITU5
P	158	SER	CYS	engineered mutation	UNP G7ITU5

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



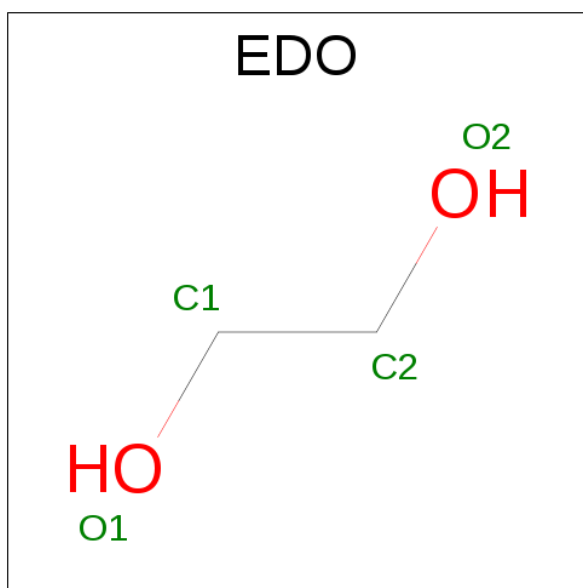
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 6	C 3	O 3	0	0
2	A	1	Total 6	C 3	O 3	0	0
2	B	1	Total 6	C 3	O 3	0	0
2	B	1	Total 6	C 3	O 3	0	0
2	B	1	Total 6	C 3	O 3	0	0
2	B	1	Total 6	C 3	O 3	0	0
2	B	1	Total 6	C 3	O 3	0	0
2	C	1	Total 6	C 3	O 3	0	0
2	C	1	Total 6	C 3	O 3	0	0
2	C	1	Total 6	C 3	O 3	0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

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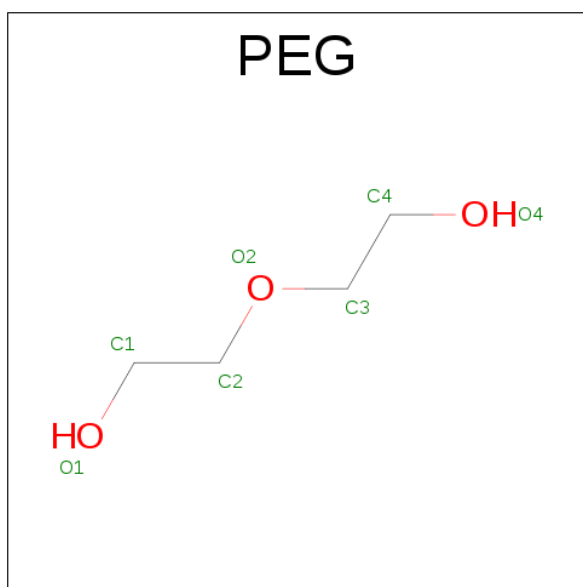
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	G	1	Total	C	O	0	0
			6	3	3		
2	G	1	Total	C	O	0	0
			6	3	3		
2	I	1	Total	C	O	0	0
			6	3	3		
2	I	1	Total	C	O	0	0
			6	3	3		
2	J	1	Total	C	O	0	0
			6	3	3		
2	J	1	Total	C	O	0	0
			6	3	3		
2	K	1	Total	C	O	0	0
			6	3	3		
2	K	1	Total	C	O	0	0
			6	3	3		
2	K	1	Total	C	O	0	0
			6	3	3		
2	L	1	Total	C	O	0	0
			6	3	3		
2	L	1	Total	C	O	0	0
			6	3	3		
2	L	1	Total	C	O	0	0
			6	3	3		
2	M	1	Total	C	O	0	0
			6	3	3		
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	N	1	Total	C	O	0	0
			6	3	3		
2	O	1	Total	C	O	0	0
			6	3	3		
2	P	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	I	1	Total	C	O	0	0
			4	2	2		
3	K	1	Total	C	O	0	0
			4	2	2		
3	L	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	140	Total	O	0	0
			140	140		
5	B	219	Total	O	0	0
			219	219		
5	C	256	Total	O	0	0
			256	256		
5	D	256	Total	O	0	0
			256	256		
5	E	242	Total	O	0	0
			242	242		
5	F	151	Total	O	0	0
			151	151		
5	G	87	Total	O	0	0
			87	87		
5	H	23	Total	O	0	0
			23	23		

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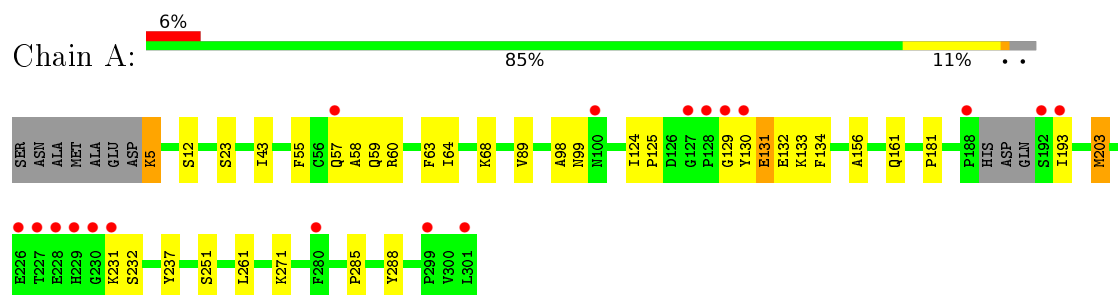
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	I	183	Total 183	O 183	0	0
5	J	238	Total 238	O 238	0	0
5	K	220	Total 220	O 220	0	0
5	L	253	Total 253	O 253	0	0
5	M	239	Total 239	O 239	0	0
5	N	252	Total 252	O 252	0	0
5	O	160	Total 160	O 160	0	0
5	P	90	Total 90	O 90	0	0

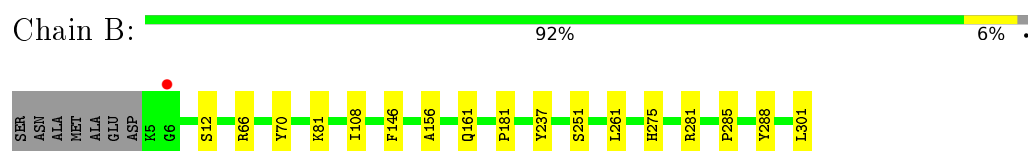
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

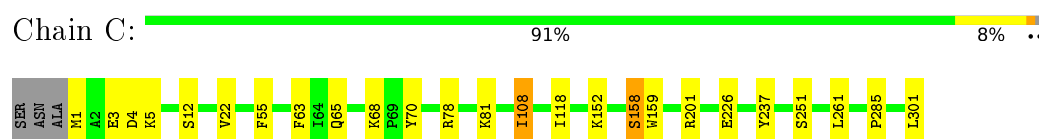
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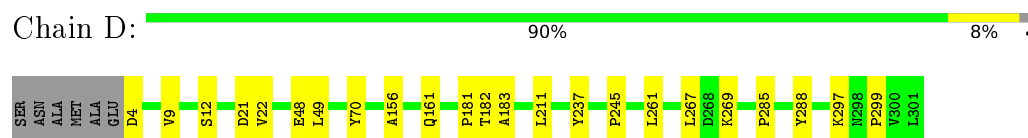
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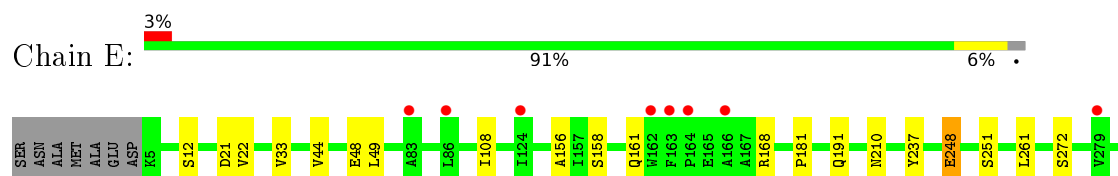
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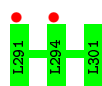


- Molecule 1: N-carbamoylputrescine amidohydrolase

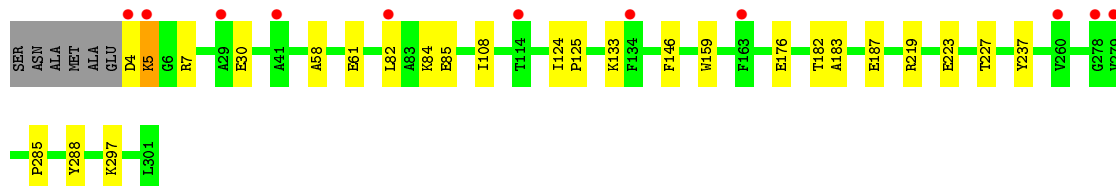
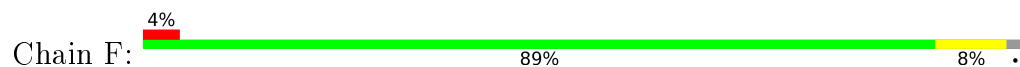


- Molecule 1: N-carbamoylputrescine amidohydrolase

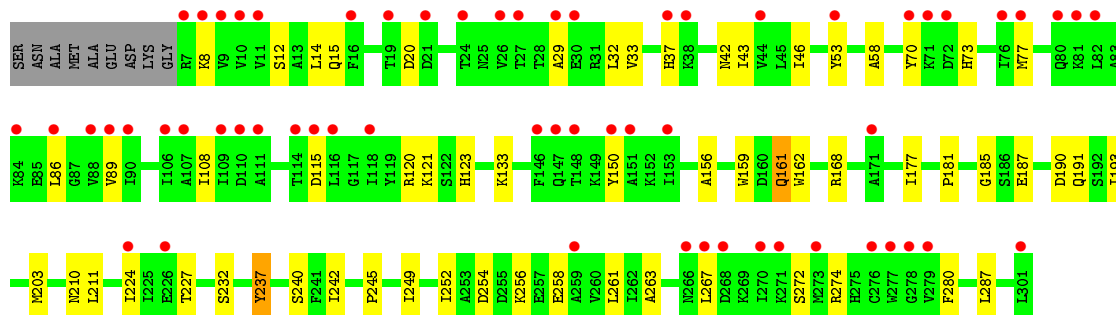
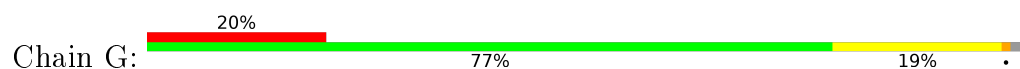




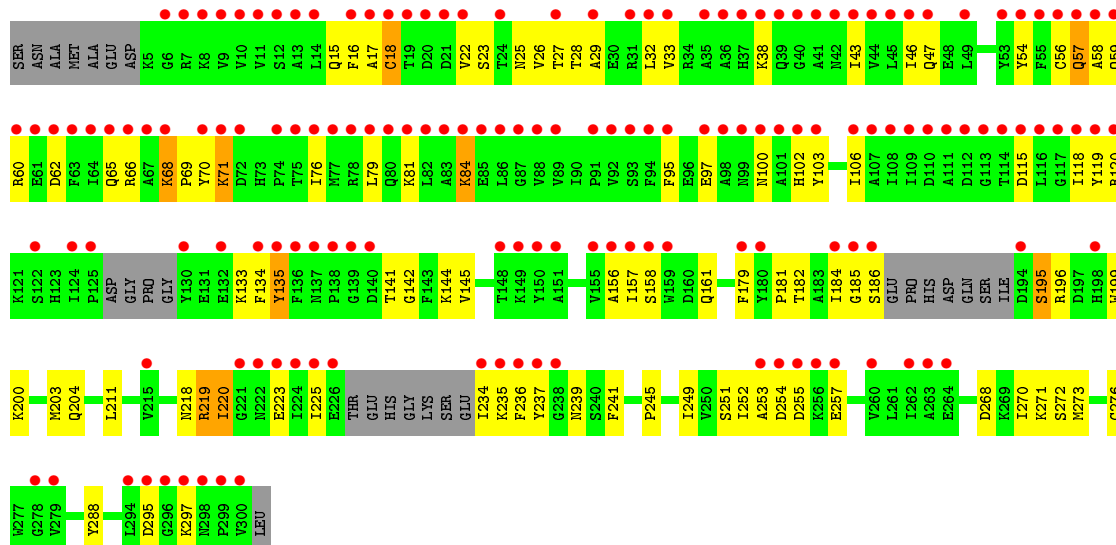
- Molecule 1: N-carbamoylputrescine amidohydrolase



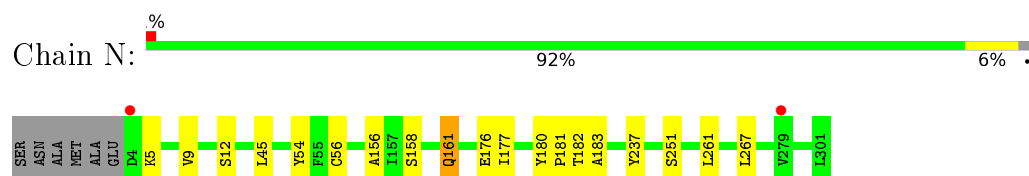
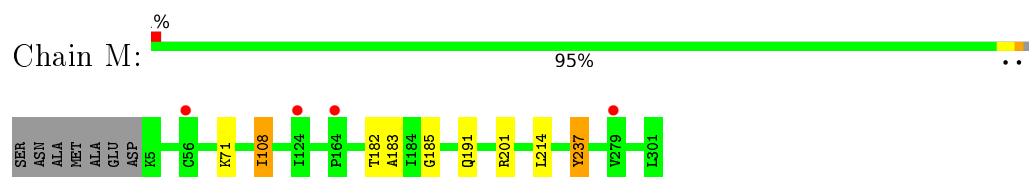
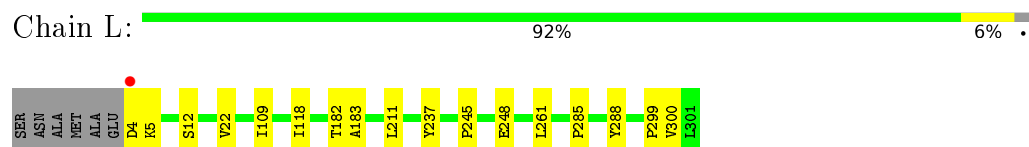
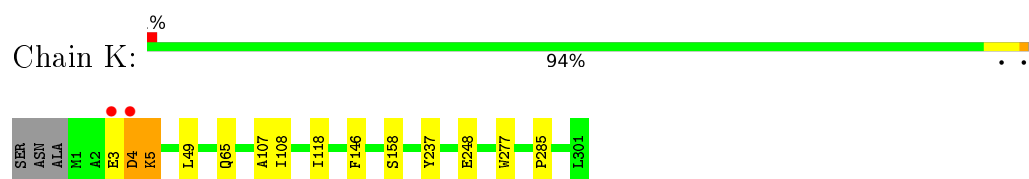
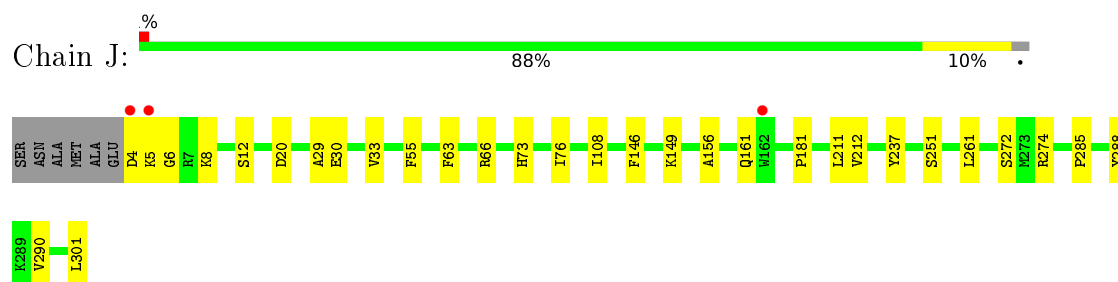
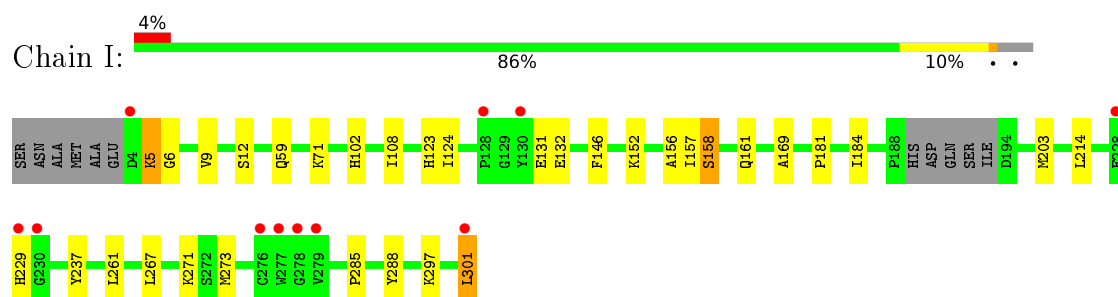
- Molecule 1: N-carbamoylputrescine amidohydrolase

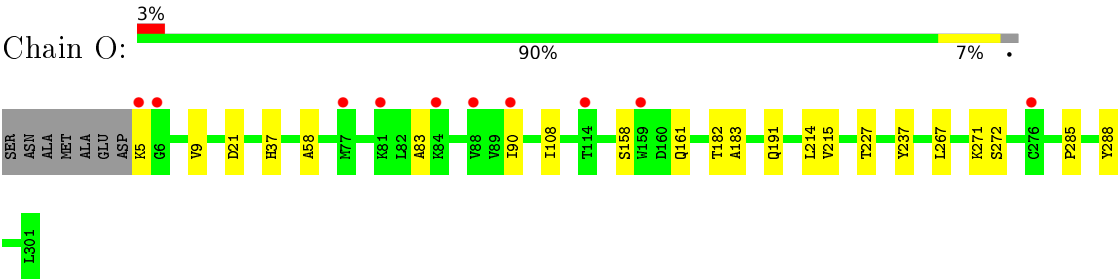


- Molecule 1: N-carbamoylputrescine amidohydrolase

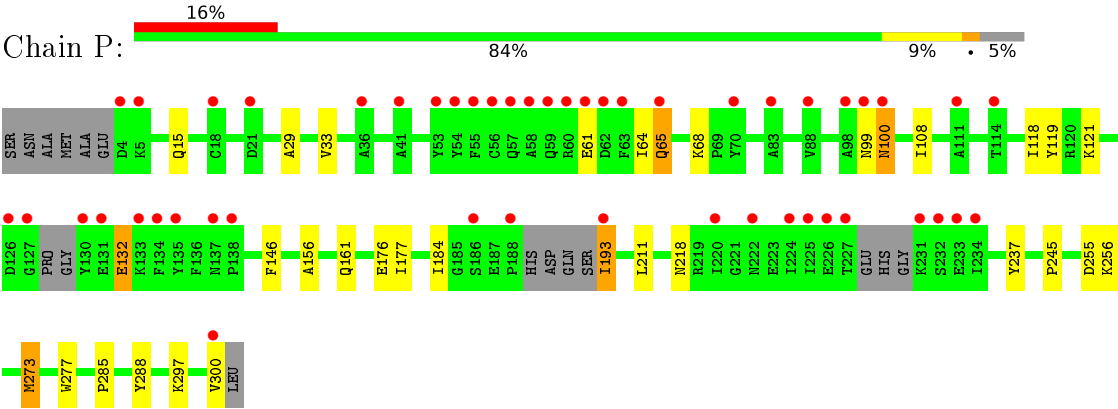


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● Molecule 1: N-carbamoylputrescine amidohydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	152.53Å 210.76Å 208.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.43 – 2.39 49.43 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.43-2.39) 99.3 (49.43-2.39)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.158 , 0.212 0.170 , 0.218	Depositor DCC
R_{free} test set	2615 reflections (1.01%)	DCC
Wilson B-factor (Å ²)	33.0	Xtriage
Anisotropy	0.685	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.1	EDS
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	2 of 261455 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	40889	wwPDB-VP
Average B, all atoms (Å ²)	57.0	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 42.31 % 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 2.0771e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.78	0/2390	0.84	0/3231
1	B	0.80	0/2422	0.82	0/3276
1	C	0.81	0/2449	0.85	0/3312
1	D	0.84	1/2427 (0.0%)	0.83	0/3283
1	E	0.76	0/2413	0.82	0/3264
1	F	0.72	0/2427	0.80	0/3283
1	G	0.80	0/2400	0.81	0/3248
1	H	0.67	0/2269	0.74	0/3065
1	I	0.81	0/2384	0.85	0/3223
1	J	0.83	0/2427	0.83	0/3283
1	K	0.81	0/2458	0.83	0/3324
1	L	0.84	0/2427	0.84	0/3283
1	M	0.79	0/2419	0.79	0/3272
1	N	0.82	0/2421	0.82	0/3275
1	O	0.76	0/2413	0.77	0/3264
1	P	0.68	0/2339	0.76	0/3160
All	All	0.78	1/38485 (0.0%)	0.81	0/52046

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	70	TYR	CG-CD1	5.09	1.45	1.39

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	2333	0	2304	25	0
1	B	2363	0	2325	8	0
1	C	2390	0	2351	14	0
1	D	2368	0	2328	10	0
1	E	2357	0	2319	8	0
1	F	2368	0	2328	18	0
1	G	2344	0	2303	37	0
1	H	2217	0	2198	81	0
1	I	2327	0	2292	20	0
1	J	2368	0	2328	17	0
1	K	2396	0	2357	12	0
1	L	2368	0	2328	11	0
1	M	2360	0	2324	7	0
1	N	2365	0	2323	9	0
1	O	2357	0	2319	10	0
1	P	2289	0	2259	19	0
2	A	12	0	16	0	0
2	B	30	0	40	1	0
2	C	18	0	24	0	0
2	D	24	0	32	1	0
2	E	24	0	32	0	0
2	F	18	0	24	2	0
2	G	18	0	24	1	0
2	I	12	0	16	0	0
2	J	12	0	16	1	0
2	K	18	0	24	1	0
2	L	18	0	24	0	0
2	M	18	0	24	0	0
2	N	24	0	32	0	0
2	O	6	0	8	1	0
2	P	6	0	8	2	0
3	A	4	0	6	1	0
3	C	4	0	6	1	0
3	D	4	0	6	0	0
3	I	4	0	6	0	0
3	K	4	0	6	2	0
3	L	4	0	6	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	7	0	10	0	0
4	G	7	0	10	0	0
4	J	7	0	10	0	0
4	L	7	0	10	0	0
5	A	140	0	0	2	0
5	B	219	0	0	3	0
5	C	256	0	0	5	0
5	D	256	0	0	3	0
5	E	242	0	0	4	0
5	F	151	0	0	1	0
5	G	87	0	0	1	0
5	H	23	0	0	1	0
5	I	183	0	0	1	0
5	J	238	0	0	5	0
5	K	220	0	0	2	0
5	L	253	0	0	4	0
5	M	239	0	0	3	0
5	N	252	0	0	1	0
5	O	160	0	0	1	0
5	P	90	0	0	1	0
All	All	40889	0	37406	300	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 4.

The worst 5 of 300 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:H:60:ARG:HG2	1:H:62:ASP:HB2	1.21	1.19
1:G:20:ASP:HB2	1:G:53:TYR:CE2	1.95	1.00
1:H:196:ARG:HB3	1:H:237:TYR:CE1	1.97	0.98
2:O:401:GOL:H12	5:P:527:HOH:O	1.64	0.97
1:H:196:ARG:HB3	1:H:237:TYR:CZ	2.00	0.96

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	291/304 (96%)	278 (96%)	13 (4%)	0	100	100
1	B	296/304 (97%)	287 (97%)	9 (3%)	0	100	100
1	C	300/304 (99%)	283 (94%)	17 (6%)	0	100	100
1	D	297/304 (98%)	287 (97%)	10 (3%)	0	100	100
1	E	295/304 (97%)	285 (97%)	10 (3%)	0	100	100
1	F	297/304 (98%)	285 (96%)	12 (4%)	0	100	100
1	G	293/304 (96%)	270 (92%)	23 (8%)	0	100	100
1	H	271/304 (89%)	244 (90%)	27 (10%)	0	100	100
1	I	290/304 (95%)	278 (96%)	12 (4%)	0	100	100
1	J	297/304 (98%)	288 (97%)	9 (3%)	0	100	100
1	K	301/304 (99%)	293 (97%)	8 (3%)	0	100	100
1	L	297/304 (98%)	289 (97%)	8 (3%)	0	100	100
1	M	296/304 (97%)	286 (97%)	10 (3%)	0	100	100
1	N	296/304 (97%)	284 (96%)	12 (4%)	0	100	100
1	O	295/304 (97%)	281 (95%)	14 (5%)	0	100	100
1	P	280/304 (92%)	267 (95%)	13 (5%)	0	100	100
All	All	4692/4864 (96%)	4485 (96%)	207 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	245/252 (97%)	233 (95%)	12 (5%)	31	48
1	B	248/252 (98%)	243 (98%)	5 (2%)	63	81
1	C	251/252 (100%)	242 (96%)	9 (4%)	42	63
1	D	249/252 (99%)	245 (98%)	4 (2%)	70	86
1	E	247/252 (98%)	239 (97%)	8 (3%)	46	68
1	F	249/252 (99%)	246 (99%)	3 (1%)	78	90
1	G	246/252 (98%)	239 (97%)	7 (3%)	51	72
1	H	232/252 (92%)	207 (89%)	25 (11%)	8	11
1	I	244/252 (97%)	236 (97%)	8 (3%)	45	66
1	J	249/252 (99%)	242 (97%)	7 (3%)	51	72
1	K	252/252 (100%)	248 (98%)	4 (2%)	70	86
1	L	249/252 (99%)	247 (99%)	2 (1%)	86	94
1	M	248/252 (98%)	246 (99%)	2 (1%)	86	94
1	N	248/252 (98%)	243 (98%)	5 (2%)	63	81
1	O	247/252 (98%)	240 (97%)	7 (3%)	51	72
1	P	240/252 (95%)	228 (95%)	12 (5%)	30	48
All	All	3944/4032 (98%)	3824 (97%)	120 (3%)	47	70

5 of 120 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	65	GLN
1	H	145	VAL
1	P	100	ASN
1	H	68	LYS
1	H	95	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	25	ASN
1	I	161	GLN
1	P	65	GLN
1	H	161	GLN
1	H	204	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 ⓘ

53 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GOL	A	401	-	5,5,5	0.54	0	5,5,5	0.43	0
2	GOL	A	402	-	5,5,5	0.34	0	5,5,5	0.43	0
3	EDO	A	403	-	3,3,3	0.50	0	2,2,2	0.24	0
2	GOL	B	401	-	5,5,5	0.94	0	5,5,5	0.70	0
2	GOL	B	402	-	5,5,5	0.25	0	5,5,5	0.45	0
2	GOL	B	403	-	5,5,5	0.53	0	5,5,5	0.75	0
2	GOL	B	404	-	5,5,5	0.31	0	5,5,5	0.52	0
2	GOL	B	405	-	5,5,5	0.64	0	5,5,5	0.45	0
2	GOL	C	401	-	5,5,5	1.15	0	5,5,5	0.82	0
2	GOL	C	402	-	5,5,5	0.32	0	5,5,5	0.29	0
2	GOL	C	403	-	5,5,5	0.50	0	5,5,5	0.74	0
4	PEG	C	404	-	6,6,6	0.64	0	5,5,5	0.40	0
3	EDO	C	405	-	3,3,3	0.48	0	2,2,2	0.36	0
2	GOL	D	401	-	5,5,5	0.91	0	5,5,5	0.77	0
2	GOL	D	402	-	5,5,5	0.29	0	5,5,5	0.28	0
2	GOL	D	403	-	5,5,5	0.47	0	5,5,5	0.37	0
2	GOL	D	404	-	5,5,5	0.68	0	5,5,5	0.55	0
3	EDO	D	405	-	3,3,3	0.61	0	2,2,2	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	E	401	-	5,5,5	1.14	0	5,5,5	0.92	0
2	GOL	E	402	-	5,5,5	0.46	0	5,5,5	0.68	0
2	GOL	E	403	-	5,5,5	0.32	0	5,5,5	0.25	0
2	GOL	E	404	-	5,5,5	0.51	0	5,5,5	0.37	0
2	GOL	F	401	-	5,5,5	0.83	0	5,5,5	0.69	0
2	GOL	F	402	-	5,5,5	0.36	0	5,5,5	0.41	0
2	GOL	F	403	-	5,5,5	0.41	0	5,5,5	0.34	0
2	GOL	G	401	-	5,5,5	0.61	0	5,5,5	0.50	0
2	GOL	G	402	-	5,5,5	0.39	0	5,5,5	0.42	0
2	GOL	G	403	-	5,5,5	0.35	0	5,5,5	0.26	0
4	PEG	G	404	-	6,6,6	0.55	0	5,5,5	0.29	0
2	GOL	I	401	-	5,5,5	0.39	0	5,5,5	0.76	0
2	GOL	I	402	-	5,5,5	0.48	0	5,5,5	0.41	0
3	EDO	I	403	-	3,3,3	0.55	0	2,2,2	0.04	0
2	GOL	J	401	-	5,5,5	0.41	0	5,5,5	0.60	0
2	GOL	J	402	-	5,5,5	0.41	0	5,5,5	0.45	0
4	PEG	J	403	-	6,6,6	0.62	0	5,5,5	0.26	0
2	GOL	K	401	-	5,5,5	1.01	0	5,5,5	0.57	0
2	GOL	K	402	-	5,5,5	0.35	0	5,5,5	0.32	0
2	GOL	K	403	-	5,5,5	0.44	0	5,5,5	0.24	0
3	EDO	K	404	-	3,3,3	0.44	0	2,2,2	0.42	0
2	GOL	L	401	-	5,5,5	0.99	0	5,5,5	0.94	0
2	GOL	L	402	-	5,5,5	0.31	0	5,5,5	0.18	0
2	GOL	L	403	-	5,5,5	0.44	0	5,5,5	0.33	0
4	PEG	L	404	-	6,6,6	0.56	0	5,5,5	0.29	0
3	EDO	L	405	-	3,3,3	0.47	0	2,2,2	0.33	0
2	GOL	M	401	-	5,5,5	0.92	0	5,5,5	1.05	0
2	GOL	M	402	-	5,5,5	0.22	0	5,5,5	0.19	0
2	GOL	M	403	-	5,5,5	0.40	0	5,5,5	0.54	0
2	GOL	N	401	-	5,5,5	0.69	0	5,5,5	0.59	0
2	GOL	N	402	-	5,5,5	0.57	0	5,5,5	0.44	0
2	GOL	N	403	-	5,5,5	0.42	0	5,5,5	0.40	0
2	GOL	N	404	-	5,5,5	0.62	0	5,5,5	0.72	0
2	GOL	O	401	-	5,5,5	0.47	0	5,5,5	0.74	0
2	GOL	P	401	-	5,5,5	0.26	0	5,5,5	0.67	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	401	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	402	-	-	0/4/4/4	0/0/0/0
3	EDO	A	403	-	-	0/1/1/1	0/0/0/0
2	GOL	B	401	-	-	0/4/4/4	0/0/0/0
2	GOL	B	402	-	-	0/4/4/4	0/0/0/0
2	GOL	B	403	-	-	0/4/4/4	0/0/0/0
2	GOL	B	404	-	-	0/4/4/4	0/0/0/0
2	GOL	B	405	-	-	0/4/4/4	0/0/0/0
2	GOL	C	401	-	-	0/4/4/4	0/0/0/0
2	GOL	C	402	-	-	0/4/4/4	0/0/0/0
2	GOL	C	403	-	-	0/4/4/4	0/0/0/0
4	PEG	C	404	-	-	0/4/4/4	0/0/0/0
3	EDO	C	405	-	-	0/1/1/1	0/0/0/0
2	GOL	D	401	-	-	0/4/4/4	0/0/0/0
2	GOL	D	402	-	-	0/4/4/4	0/0/0/0
2	GOL	D	403	-	-	0/4/4/4	0/0/0/0
2	GOL	D	404	-	-	0/4/4/4	0/0/0/0
3	EDO	D	405	-	-	0/1/1/1	0/0/0/0
2	GOL	E	401	-	-	0/4/4/4	0/0/0/0
2	GOL	E	402	-	-	0/4/4/4	0/0/0/0
2	GOL	E	403	-	-	0/4/4/4	0/0/0/0
2	GOL	E	404	-	-	0/4/4/4	0/0/0/0
2	GOL	F	401	-	-	0/4/4/4	0/0/0/0
2	GOL	F	402	-	-	0/4/4/4	0/0/0/0
2	GOL	F	403	-	-	0/4/4/4	0/0/0/0
2	GOL	G	401	-	-	0/4/4/4	0/0/0/0
2	GOL	G	402	-	-	0/4/4/4	0/0/0/0
2	GOL	G	403	-	-	0/4/4/4	0/0/0/0
4	PEG	G	404	-	-	0/4/4/4	0/0/0/0
2	GOL	I	401	-	-	0/4/4/4	0/0/0/0
2	GOL	I	402	-	-	0/4/4/4	0/0/0/0
3	EDO	I	403	-	-	0/1/1/1	0/0/0/0
2	GOL	J	401	-	-	0/4/4/4	0/0/0/0
2	GOL	J	402	-	-	0/4/4/4	0/0/0/0
4	PEG	J	403	-	-	0/4/4/4	0/0/0/0
2	GOL	K	401	-	-	0/4/4/4	0/0/0/0
2	GOL	K	402	-	-	0/4/4/4	0/0/0/0
2	GOL	K	403	-	-	0/4/4/4	0/0/0/0
3	EDO	K	404	-	-	0/1/1/1	0/0/0/0
2	GOL	L	401	-	-	0/4/4/4	0/0/0/0
2	GOL	L	402	-	-	0/4/4/4	0/0/0/0
2	GOL	L	403	-	-	0/4/4/4	0/0/0/0
4	PEG	L	404	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	L	405	-	-	0/1/1/1	0/0/0/0
2	GOL	M	401	-	-	0/4/4/4	0/0/0/0
2	GOL	M	402	-	-	0/4/4/4	0/0/0/0
2	GOL	M	403	-	-	0/4/4/4	0/0/0/0
2	GOL	N	401	-	-	0/4/4/4	0/0/0/0
2	GOL	N	402	-	-	0/4/4/4	0/0/0/0
2	GOL	N	403	-	-	0/4/4/4	0/0/0/0
2	GOL	N	404	-	-	0/4/4/4	0/0/0/0
2	GOL	O	401	-	-	0/4/4/4	0/0/0/0
2	GOL	P	401	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	403	EDO	1	0
2	B	405	GOL	1	0
3	C	405	EDO	1	0
2	D	404	GOL	1	0
2	F	401	GOL	2	0
2	G	402	GOL	1	0
2	J	402	GOL	1	0
2	K	402	GOL	1	0
3	K	404	EDO	2	0
3	L	405	EDO	2	0
2	O	401	GOL	1	0
2	P	401	GOL	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	294/304 (96%)	0.06	18 (6%) 25 25	35, 57, 105, 133	0
1	B	297/304 (97%)	-0.33	1 (0%) 94 94	32, 45, 68, 113	0
1	C	301/304 (99%)	-0.32	0 100 100	30, 42, 62, 113	0
1	D	298/304 (98%)	-0.32	0 100 100	30, 42, 60, 99	0
1	E	297/304 (97%)	0.17	10 (3%) 49 49	31, 45, 65, 99	0
1	F	298/304 (98%)	0.29	11 (3%) 45 46	32, 57, 80, 108	0
1	G	295/304 (97%)	0.99	60 (20%) 1 1	60, 90, 113, 123	0
1	H	278/304 (91%)	2.42	156 (56%) 0 0	74, 118, 143, 162	0
1	I	293/304 (96%)	-0.03	11 (3%) 44 45	34, 48, 92, 132	0
1	J	298/304 (98%)	-0.26	3 (1%) 84 83	31, 42, 62, 121	0
1	K	301/304 (99%)	-0.22	2 (0%) 89 88	31, 45, 67, 118	0
1	L	298/304 (98%)	-0.32	1 (0%) 94 94	31, 42, 59, 98	0
1	M	297/304 (97%)	0.06	4 (1%) 79 79	31, 43, 62, 87	0
1	N	298/304 (98%)	-0.21	2 (0%) 89 88	32, 42, 60, 110	0
1	O	297/304 (97%)	0.19	10 (3%) 49 49	40, 61, 82, 119	0
1	P	288/304 (94%)	0.78	49 (17%) 2 2	43, 73, 117, 132	0
All	All	4728/4864 (97%)	0.17	338 (7%) 19 19	30, 49, 110, 162	0

The worst 5 of 338 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	58	ALA	12.9
1	H	29	ALA	8.7
1	H	111	ALA	8.1
1	I	301	LEU	8.0
1	H	300	VAL	7.0

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	GOL	G	401	6/6	0.91	0.34	9.83	76,78,79,81	0
2	GOL	D	402	6/6	0.94	0.19	9.81	53,57,87,89	0
2	GOL	N	404	6/6	0.79	0.35	9.80	65,76,82,89	0
2	GOL	F	403	6/6	0.91	0.35	9.55	62,77,82,89	0
2	GOL	K	403	6/6	0.91	0.28	8.73	57,67,74,77	0
3	EDO	K	404	4/4	0.91	0.42	7.51	68,70,73,73	0
2	GOL	A	401	6/6	0.90	0.19	7.40	68,79,90,90	0
2	GOL	J	402	6/6	0.89	0.29	7.01	63,67,79,92	0
4	PEG	L	404	7/7	0.89	0.51	7.01	68,75,98,100	0
2	GOL	L	403	6/6	0.98	0.35	6.92	49,67,71,73	0
2	GOL	C	403	6/6	0.91	0.19	6.82	49,57,66,67	0
2	GOL	E	403	6/6	0.94	0.25	6.25	56,59,65,66	0
2	GOL	D	404	6/6	0.84	0.28	6.14	50,65,73,85	0
2	GOL	E	404	6/6	0.70	0.48	5.74	73,85,99,100	0
2	GOL	E	401	6/6	0.92	0.36	4.97	49,52,55,55	0
2	GOL	N	403	6/6	0.95	0.20	4.92	49,61,64,72	0
2	GOL	M	401	6/6	0.90	0.31	4.63	50,54,56,59	0
2	GOL	D	403	6/6	0.93	0.31	4.46	54,61,67,70	0
2	GOL	G	403	6/6	0.92	0.32	4.43	61,73,84,85	0
2	GOL	L	401	6/6	0.94	0.34	4.42	51,60,62,73	0
2	GOL	M	403	6/6	0.94	0.22	4.17	53,62,70,72	0
2	GOL	O	401	6/6	0.91	0.34	4.03	62,67,69,70	0
3	EDO	C	405	4/4	0.92	0.31	3.81	65,69,71,79	0
2	GOL	N	401	6/6	0.89	0.29	3.74	57,60,64,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	GOL	L	402	6/6	0.96	0.19	3.44	62,68,83,91	0
3	EDO	I	403	4/4	0.95	0.27	3.39	58,62,66,77	0
2	GOL	C	402	6/6	0.97	0.18	3.24	52,58,85,90	0
2	GOL	J	401	6/6	0.93	0.29	3.19	49,53,53,54	0
2	GOL	B	401	6/6	0.93	0.24	2.76	49,52,55,55	0
3	EDO	D	405	4/4	0.93	0.22	2.60	60,65,72,76	0
3	EDO	A	403	4/4	0.95	0.26	2.37	64,64,67,74	0
2	GOL	F	401	6/6	0.88	0.26	2.30	71,74,76,77	0
2	GOL	G	402	6/6	0.89	0.21	2.27	75,82,95,100	0
2	GOL	C	401	6/6	0.92	0.18	2.16	46,49,51,54	0
2	GOL	B	404	6/6	0.91	0.15	2.00	61,68,71,74	0
3	EDO	L	405	4/4	0.95	0.19	1.78	52,67,69,71	0
2	GOL	K	401	6/6	0.92	0.16	1.70	49,52,55,56	0
2	GOL	I	401	6/6	0.94	0.23	1.44	48,55,67,79	0
2	GOL	N	402	6/6	0.92	0.18	1.37	47,74,97,98	0
2	GOL	E	402	6/6	0.90	0.18	1.32	63,66,76,78	0
2	GOL	F	402	6/6	0.96	0.20	1.24	54,66,78,84	0
2	GOL	D	401	6/6	0.95	0.22	1.24	49,51,54,63	0
2	GOL	K	402	6/6	0.97	0.15	0.72	52,59,81,84	0
2	GOL	M	402	6/6	0.97	0.13	0.64	52,61,68,85	0
2	GOL	B	402	6/6	0.97	0.16	0.52	44,60,65,85	0
2	GOL	I	402	6/6	0.94	0.10	0.42	61,68,75,76	0
2	GOL	B	403	6/6	0.92	0.14	0.16	52,72,79,85	0
2	GOL	A	402	6/6	0.95	0.13	-0.51	55,65,69,72	0
2	GOL	P	401	6/6	0.95	0.12	-1.27	53,63,66,68	0
4	PEG	G	404	7/7	0.81	0.21	-1.29	73,89,99,102	0
2	GOL	B	405	6/6	0.65	0.45	-	62,68,87,87	0
4	PEG	J	403	7/7	0.80	0.38	-	74,97,101,102	0
4	PEG	C	404	7/7	0.87	0.33	-	68,102,116,120	0

6.5 Other polymers

There are no such residues in this entry.