



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 06:34 PM UTC

PDB ID : 5H8J / pdb_00005h8j
Title : Crystal structure of Medicago truncatula N-carbamoylputrescine amidohydrolase (MtCPA) in complex with cadaverine
Authors : Sekula, B.; Ruszkowski, M.; Malinska, M.; Dauter, Z.
Deposited on : 2015-12-23
Resolution : 2.19 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

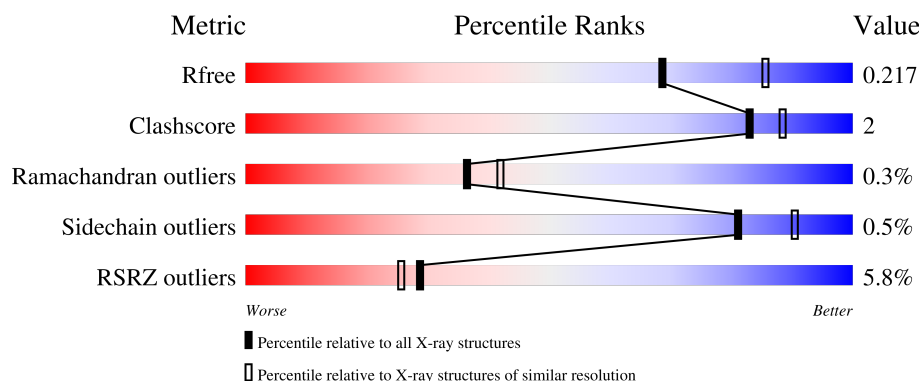
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	304	7% 88% 8% ..
1	B	304	% 92% 5% ..
1	C	304	% 96% ..
1	D	304	91% 6% ..
1	E	304	91% 6% ..

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Mol	Chain	Length	Quality of chain
1	F	304	% 91% 6% ..
1	G	304	18% 86% 11% ..
1	H	304	43% 77% 11% 12%
1	I	304	4% 85% 11% .
1	J	304	% 91% 6% ..
1	K	304	% 94% ..
1	L	304	93% 5% .
1	M	304	% 91% 6% .
1	N	304	% 94% ..
1	O	304	2% 90% 8% .
1	P	304	9% 87% 5% 8%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 41003 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
			2360	1508	407	435	10			
1	B	297	Total	C	N	O	S	0	0	0
			2357	1505	408	436	8			
1	C	301	Total	C	N	O	S	0	1	0
			2390	1524	412	444	10			
1	D	298	Total	C	N	O	S	0	3	0
			2382	1522	409	443	8			
1	E	297	Total	C	N	O	S	0	0	0
			2357	1505	408	436	8			
1	F	298	Total	C	N	O	S	0	0	0
			2365	1509	409	439	8			
1	G	295	Total	C	N	O	S	0	0	0
			2344	1497	405	434	8			
1	H	268	Total	C	N	O	S	0	0	0
			2131	1368	371	384	8			
1	I	292	Total	C	N	O	S	0	1	0
			2322	1484	400	429	9			
1	J	298	Total	C	N	O	S	0	1	0
			2369	1513	409	439	8			
1	K	301	Total	C	N	O	S	0	0	0
			2387	1522	412	444	9			
1	L	298	Total	C	N	O	S	0	2	0
			2374	1515	409	441	9			
1	M	298	Total	C	N	O	S	0	0	0
			2365	1509	409	439	8			
1	N	298	Total	C	N	O	S	0	1	0
			2369	1513	409	439	8			
1	O	298	Total	C	N	O	S	0	1	0
			2371	1513	409	441	8			
1	P	279	Total	C	N	O	S	0	1	0
			2217	1421	384	403	9			

There are 48 discrepancies between the modelled and reference sequences:

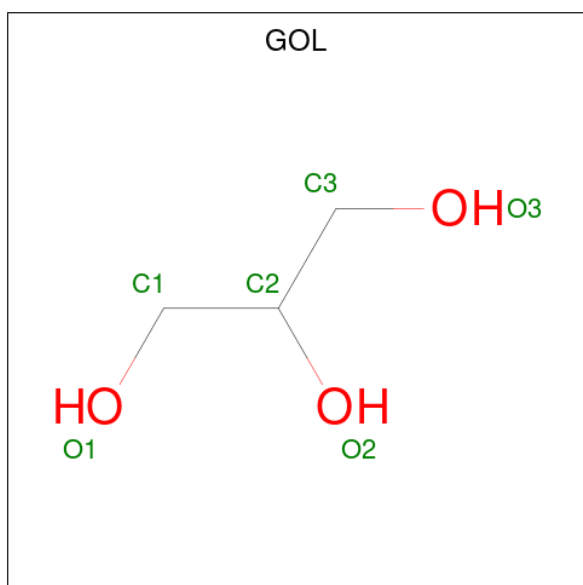
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP G7ITU5
A	-1	ASN	-	expression tag	UNP G7ITU5
A	0	ALA	-	expression tag	UNP G7ITU5
B	-2	SER	-	expression tag	UNP G7ITU5
B	-1	ASN	-	expression tag	UNP G7ITU5
B	0	ALA	-	expression tag	UNP G7ITU5
C	-2	SER	-	expression tag	UNP G7ITU5
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 (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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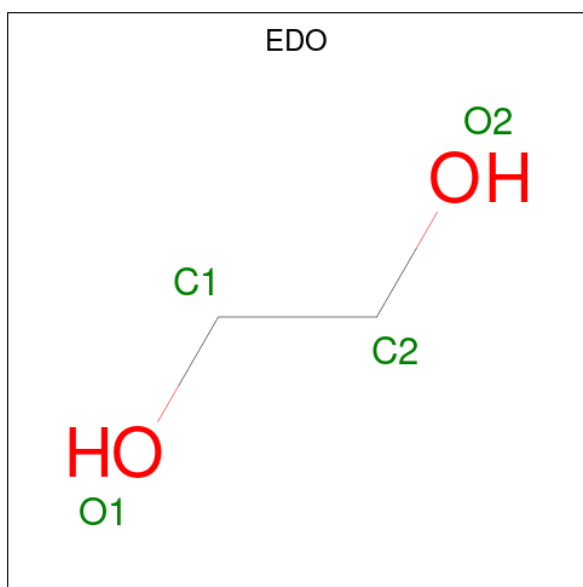
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	G	1	Total	C	O	0	0
			6	3	3		
2	H	1	Total	C	O	0	0
			6	3	3		
2	I	1	Total	C	O	0	0
			6	3	3		
2	I	1	Total	C	O	0	0
			6	3	3		
2	I	1	Total	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	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	O	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 (CCD ID: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



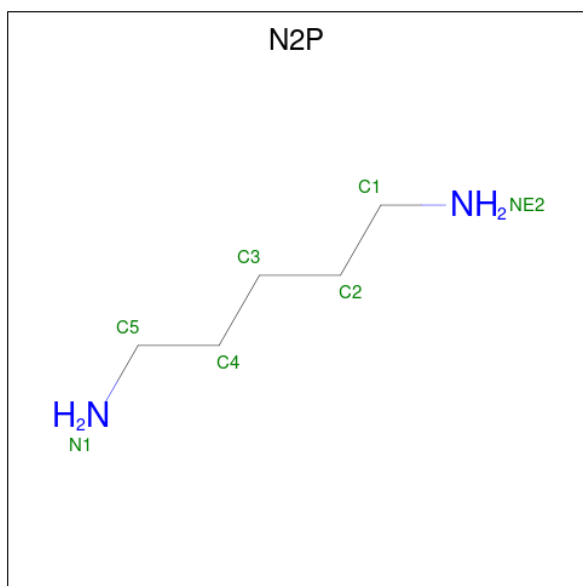
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	I	1	Total C O 4 2 2	0	0
4	J	1	Total C O 4 2 2	0	0
4	K	1	Total C O 4 2 2	0	0
4	L	1	Total C O 4 2 2	0	0
4	N	1	Total C O 4 2 2	0	0

- Molecule 5 is PENTANE-1,5-DIAMINE (CCD ID: N2P) (formula: C₅H₁₄N₂).



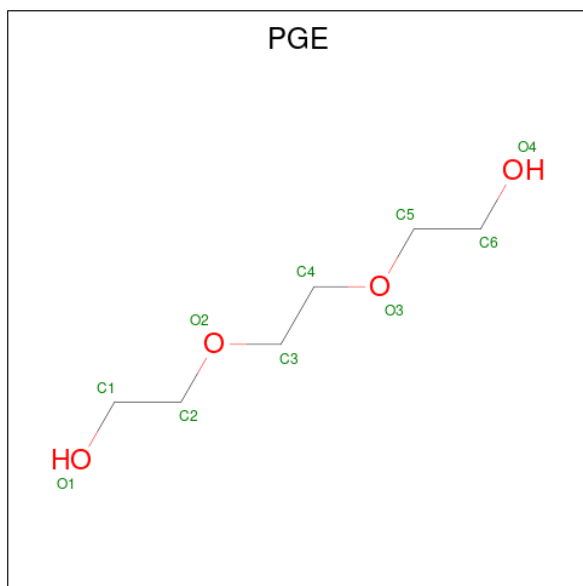
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C N 7 5 2	0	0
5	C	1	Total C N 7 5 2	0	0
5	D	1	Total C N 7 5 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	C	N	0	0
			7	5	2		
5	F	1	Total	C	N	0	0
			7	5	2		
5	G	1	Total	C	N	0	0
			7	5	2		
5	J	1	Total	C	N	0	0
			7	5	2		
5	K	1	Total	C	N	0	0
			7	5	2		
5	L	1	Total	C	N	0	0
			7	5	2		
5	M	1	Total	C	N	0	0
			7	5	2		
5	N	1	Total	C	N	0	0
			7	5	2		
5	O	1	Total	C	N	0	0
			7	5	2		

- Molecule 6 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			10	6	4		

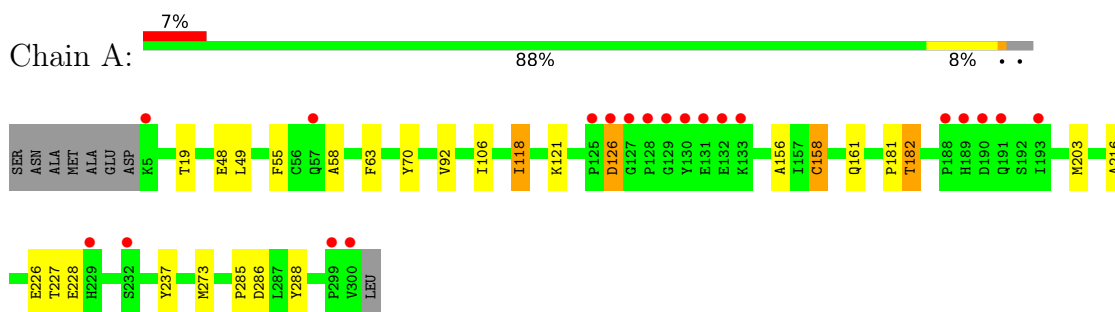
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	157	Total 157	O 157	0	0
7	B	233	Total 233	O 233	0	0
7	C	258	Total 258	O 258	0	0
7	D	288	Total 288	O 288	0	0
7	E	236	Total 236	O 236	0	0
7	F	177	Total 177	O 177	0	0
7	G	120	Total 120	O 120	0	0
7	H	38	Total 38	O 38	0	0
7	I	171	Total 171	O 171	0	0
7	J	232	Total 232	O 232	0	0
7	K	241	Total 241	O 241	0	0
7	L	277	Total 277	O 277	0	0
7	M	263	Total 263	O 263	0	0
7	N	253	Total 253	O 253	0	0
7	O	206	Total 206	O 206	0	0
7	P	92	Total 92	O 92	0	0

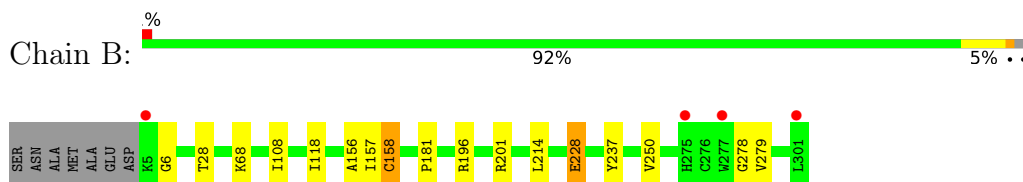
3 Residue-property plots [i](#)

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

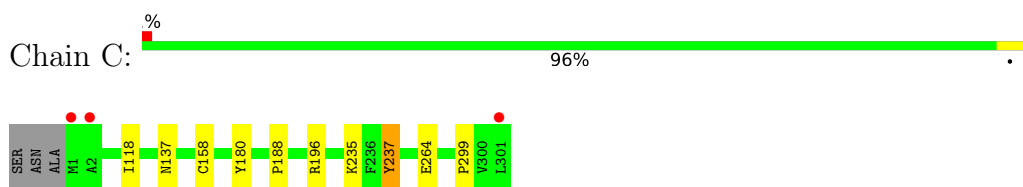
- Molecule 1: N-carbamoylputrescine amidohydrolase



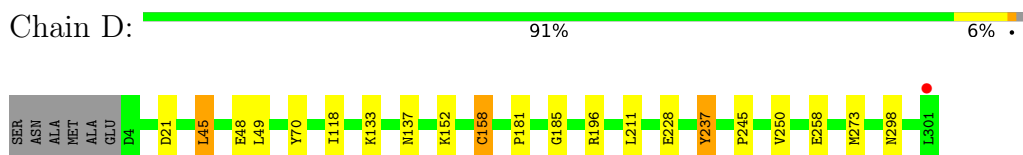
- Molecule 1: N-carbamoylputrescine amidohydrolase



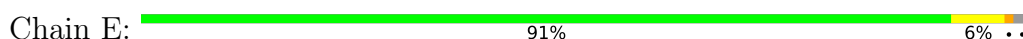
- Molecule 1: N-carbamoylputrescine amidohydrolase



- Molecule 1: N-carbamoylputrescine amidohydrolase



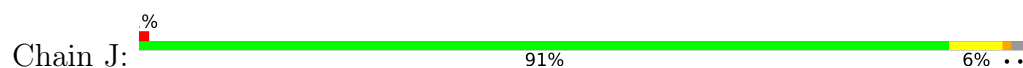
- Molecule 1: N-carbamoylputrescine amidohydrolase







- Molecule 1: N-carbamoylputrescine amidohydrolase



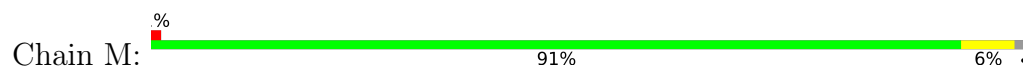
- Molecule 1: N-carbamoylputrescine amidohydrolase



- Molecule 1: N-carbamoylputrescine amidohydrolase



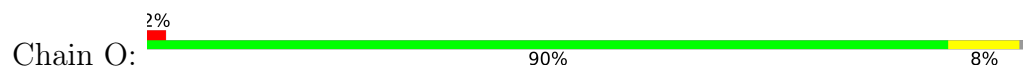
- Molecule 1: N-carbamoylputrescine amidohydrolase



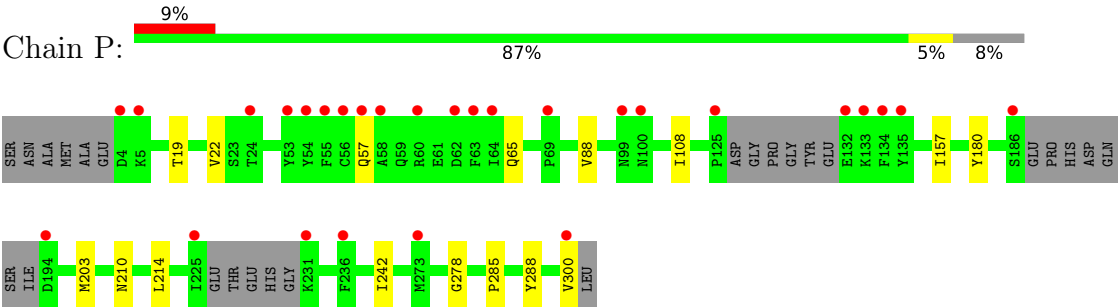
- Molecule 1: N-carbamoylputrescine amidohydrolase



- 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, α , β , γ	152.27Å 211.04Å 208.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.56 – 2.19 39.56 – 2.19	Depositor EDS
% Data completeness (in resolution range)	99.1 (39.56-2.19) 99.1 (39.56-2.19)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.171 , 0.211 0.181 , 0.217	Depositor DCC
R_{free} test set	3402 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.469	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	41003	wwPDB-VP
Average B, all atoms (Å ²)	52.0	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 41.46 % 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 2.3540e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: N2P, GOL, PEG, EDO, PGE

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	1.17	3/2425 (0.1%)	1.02	4/3281 (0.1%)
1	B	1.22	3/2413 (0.1%)	1.02	6/3264 (0.2%)
1	C	1.21	3/2449 (0.1%)	1.01	4/3312 (0.1%)
1	D	1.28	4/2447 (0.2%)	1.06	6/3310 (0.2%)
1	E	1.18	2/2413 (0.1%)	1.01	3/3264 (0.1%)
1	F	1.12	2/2421 (0.1%)	1.00	5/3275 (0.2%)
1	G	1.29	9/2400 (0.4%)	1.05	6/3248 (0.2%)
1	H	1.18	2/2179 (0.1%)	1.03	7/2944 (0.2%)
1	I	1.22	5/2378 (0.2%)	1.05	9/3213 (0.3%)
1	J	1.25	3/2428 (0.1%)	1.04	5/3285 (0.2%)
1	K	1.17	2/2443 (0.1%)	1.00	4/3304 (0.1%)
1	L	1.24	4/2436 (0.2%)	1.03	5/3295 (0.2%)
1	M	1.19	3/2421 (0.1%)	1.02	4/3275 (0.1%)
1	N	1.22	0/2428	1.01	5/3285 (0.2%)
1	O	1.24	5/2430 (0.2%)	1.00	6/3287 (0.2%)
1	P	1.07	2/2268 (0.1%)	0.96	4/3063 (0.1%)
All	All	1.20	52/38379 (0.1%)	1.02	83/51905 (0.2%)

The worst 5 of 52 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	126	ASP	CA-C	8.98	1.61	1.53
1	L	249	ILE	C-O	-8.54	1.15	1.24
1	K	252	ILE	C-O	-7.34	1.15	1.23
1	O	215	VAL	C-O	7.18	1.31	1.24
1	J	180	TYR	CA-C	6.74	1.59	1.52

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	5	LYS	N-CA-C	7.53	121.30	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	6	GLY	N-CA-C	7.32	120.48	112.29
1	G	92	VAL	N-CA-C	6.81	117.22	106.88
1	K	237	TYR	N-CA-C	6.71	121.08	113.02
1	D	258	GLU	N-CA-C	-6.64	100.46	110.28

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	2360	0	2329	14	0
1	B	2357	0	2319	9	0
1	C	2390	0	2351	5	0
1	D	2382	0	2346	12	0
1	E	2357	0	2319	12	0
1	F	2365	0	2323	13	0
1	G	2344	0	2303	17	0
1	H	2131	0	2113	17	0
1	I	2322	0	2289	14	0
1	J	2369	0	2332	12	0
1	K	2387	0	2346	11	0
1	L	2374	0	2334	8	0
1	M	2365	0	2323	14	0
1	N	2369	0	2332	11	0
1	O	2371	0	2329	13	0
1	P	2217	0	2198	6	0
2	A	18	0	24	0	0
2	B	6	0	8	1	0
2	C	18	0	24	0	0
2	D	6	0	8	0	0
2	E	12	0	16	0	0
2	F	12	0	16	1	0
2	G	6	0	8	0	0
2	H	6	0	8	0	0
2	I	18	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	12	0	16	0	0
2	M	18	0	24	0	0
2	N	6	0	8	0	0
2	O	12	0	16	0	0
3	A	7	0	10	0	0
3	G	7	0	10	0	0
3	L	7	0	10	0	0
4	A	4	0	6	0	0
4	C	4	0	6	0	0
4	D	4	0	6	0	0
4	F	4	0	6	0	0
4	I	4	0	6	0	0
4	J	4	0	6	0	0
4	K	4	0	6	0	0
4	L	4	0	6	0	0
4	N	4	0	6	0	0
5	B	7	0	14	3	0
5	C	7	0	14	3	0
5	D	7	0	14	3	0
5	E	7	0	14	3	0
5	F	7	0	14	3	0
5	G	7	0	14	2	0
5	J	7	0	14	3	0
5	K	7	0	14	3	0
5	L	7	0	14	3	0
5	M	7	0	14	2	0
5	N	7	0	14	3	0
5	O	7	0	14	3	0
6	B	10	0	14	0	0
7	A	157	0	0	1	0
7	B	233	0	0	2	0
7	C	258	0	0	2	0
7	D	288	0	0	0	0
7	E	236	0	0	1	0
7	F	177	0	0	3	0
7	G	120	0	0	0	0
7	H	38	0	0	0	0
7	I	171	0	0	0	0
7	J	232	0	0	0	0
7	K	241	0	0	0	0
7	L	277	0	0	0	0
7	M	263	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	N	253	0	0	2	0
7	O	206	0	0	0	0
7	P	92	0	0	0	0
All	All	41003	0	37352	181	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 181 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:M:158:CYS:SG	5:M:401:N2P:H5C1	1.98	1.04
1:F:158:CYS:SG	5:F:402:N2P:H5C1	1.96	1.04
1:O:211:LEU:HD11	1:O:277:TRP:CE3	2.09	0.87
1:J:158:CYS:SG	5:J:401:N2P:H5C1	2.14	0.87
1:M:158:CYS:SG	5:M:401:N2P:C5	2.66	0.83

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	297/304 (98%)	280 (94%)	16 (5%)	1 (0%)	36	42
1	B	295/304 (97%)	286 (97%)	8 (3%)	1 (0%)	36	42
1	C	300/304 (99%)	289 (96%)	11 (4%)	0	100	100
1	D	299/304 (98%)	292 (98%)	6 (2%)	1 (0%)	36	42
1	E	295/304 (97%)	284 (96%)	10 (3%)	1 (0%)	36	42
1	F	296/304 (97%)	287 (97%)	8 (3%)	1 (0%)	36	42
1	G	293/304 (96%)	281 (96%)	11 (4%)	1 (0%)	36	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	260/304 (86%)	245 (94%)	14 (5%)	1 (0%)	30	34
1	I	289/304 (95%)	279 (96%)	10 (4%)	0	100	100
1	J	297/304 (98%)	289 (97%)	7 (2%)	1 (0%)	36	42
1	K	299/304 (98%)	290 (97%)	8 (3%)	1 (0%)	36	42
1	L	298/304 (98%)	290 (97%)	7 (2%)	1 (0%)	36	42
1	M	296/304 (97%)	285 (96%)	10 (3%)	1 (0%)	36	42
1	N	297/304 (98%)	284 (96%)	12 (4%)	1 (0%)	36	42
1	O	297/304 (98%)	282 (95%)	14 (5%)	1 (0%)	36	42
1	P	272/304 (90%)	264 (97%)	8 (3%)	0	100	100
All	All	4680/4864 (96%)	4507 (96%)	160 (3%)	13 (0%)	36	42

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	158	CYS
1	N	158	CYS
1	E	158	CYS
1	F	158	CYS
1	G	158	CYS

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%)	245 (98%)	4 (2%)	55	71
1	B	247/252 (98%)	246 (100%)	1 (0%)	84	92
1	C	251/252 (100%)	250 (100%)	1 (0%)	84	92
1	D	251/252 (100%)	250 (100%)	1 (0%)	84	92
1	E	247/252 (98%)	246 (100%)	1 (0%)	84	92
1	F	248/252 (98%)	248 (100%)	0	100	100
1	G	246/252 (98%)	245 (100%)	1 (0%)	84	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	222/252 (88%)	220 (99%)	2 (1%)	70	84
1	I	243/252 (96%)	241 (99%)	2 (1%)	73	85
1	J	249/252 (99%)	248 (100%)	1 (0%)	84	92
1	K	250/252 (99%)	248 (99%)	2 (1%)	73	85
1	L	250/252 (99%)	250 (100%)	0	100	100
1	M	248/252 (98%)	246 (99%)	2 (1%)	73	85
1	N	249/252 (99%)	248 (100%)	1 (0%)	84	92
1	O	249/252 (99%)	249 (100%)	0	100	100
1	P	232/252 (92%)	229 (99%)	3 (1%)	61	76
All	All	3931/4032 (98%)	3909 (99%)	22 (1%)	81	89

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	228	GLU
1	M	251	SER
1	M	237	TYR
1	N	228	GLU
1	D	228	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	37	HIS
1	P	204	GLN
1	L	39	GLN
1	P	137	ASN
1	O	298	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

50 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	M	404	-	5,5,5	0.42	0	5,5,5	0.11	0
4	EDO	K	404	-	3,3,3	0.52	0	2,2,2	0.21	0
5	N2P	F	402	-	6,6,6	0.48	0	5,5,5	0.69	0
2	GOL	B	402	-	5,5,5	0.50	0	5,5,5	0.46	0
2	GOL	F	401	-	5,5,5	0.30	0	5,5,5	0.49	0
3	PEG	L	402	-	6,6,6	0.60	0	5,5,5	0.25	0
2	GOL	K	402	-	5,5,5	0.24	0	5,5,5	0.21	0
2	GOL	O	402	-	5,5,5	0.19	0	5,5,5	0.75	0
5	N2P	L	401	-	6,6,6	0.28	0	5,5,5	0.59	0
2	GOL	F	403	-	5,5,5	0.50	0	5,5,5	0.22	0
2	GOL	D	402	-	5,5,5	0.81	0	5,5,5	0.50	0
2	GOL	M	402	-	5,5,5	0.38	0	5,5,5	0.30	0
4	EDO	I	404	-	3,3,3	0.54	0	2,2,2	0.25	0
2	GOL	I	401	-	5,5,5	0.37	0	5,5,5	0.32	0
2	GOL	G	403	-	5,5,5	0.33	0	5,5,5	0.60	0
2	GOL	I	403	-	5,5,5	0.47	0	5,5,5	0.26	0
2	GOL	C	402	-	5,5,5	0.57	0	5,5,5	0.29	0
4	EDO	N	403	-	3,3,3	0.53	0	2,2,2	0.16	0
2	GOL	C	403	-	5,5,5	0.45	0	5,5,5	0.27	0
5	N2P	G	401	-	6,6,6	0.35	0	5,5,5	0.80	0
4	EDO	L	403	-	3,3,3	0.72	0	2,2,2	0.03	0
4	EDO	D	403	-	3,3,3	0.59	0	2,2,2	0.19	0
2	GOL	H	401	-	5,5,5	0.67	0	5,5,5	0.58	0
5	N2P	J	401	-	6,6,6	0.23	0	5,5,5	0.84	0
5	N2P	C	401	-	6,6,6	0.20	0	5,5,5	0.93	0
4	EDO	J	402	-	3,3,3	0.41	0	2,2,2	0.44	0
5	N2P	B	401	-	6,6,6	0.24	0	5,5,5	1.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	N2P	E	401	-	6,6,6	0.25	0	5,5,5	0.41	0
2	GOL	E	402	-	5,5,5	0.54	0	5,5,5	0.34	0
3	PEG	G	402	-	6,6,6	0.63	0	5,5,5	0.37	0
2	GOL	E	403	-	5,5,5	0.37	0	5,5,5	0.27	0
2	GOL	I	402	-	5,5,5	0.52	0	5,5,5	0.37	0
2	GOL	N	402	-	5,5,5	0.49	0	5,5,5	0.24	0
6	PGE	B	403	-	9,9,9	0.59	0	8,8,8	0.28	0
4	EDO	F	404	-	3,3,3	0.58	0	2,2,2	0.22	0
5	N2P	N	401	-	6,6,6	0.47	0	5,5,5	0.39	0
4	EDO	A	405	-	3,3,3	0.69	0	2,2,2	0.17	0
5	N2P	K	401	-	6,6,6	0.30	0	5,5,5	0.88	0
2	GOL	K	403	-	5,5,5	1.05	0	5,5,5	0.90	0
2	GOL	C	404	-	5,5,5	0.53	0	5,5,5	0.22	0
2	GOL	A	404	-	5,5,5	0.56	0	5,5,5	0.38	0
2	GOL	A	402	-	5,5,5	0.39	0	5,5,5	0.50	0
4	EDO	C	405	-	3,3,3	0.59	0	2,2,2	0.16	0
2	GOL	M	403	-	5,5,5	1.33	0	5,5,5	0.76	0
2	GOL	A	401	-	5,5,5	0.76	0	5,5,5	0.43	0
5	N2P	D	401	-	6,6,6	0.29	0	5,5,5	0.49	0
5	N2P	O	401	-	6,6,6	0.55	0	5,5,5	0.81	0
2	GOL	O	403	-	5,5,5	0.47	0	5,5,5	0.12	0
3	PEG	A	403	-	6,6,6	0.64	0	5,5,5	0.27	0
5	N2P	M	401	-	6,6,6	0.43	0	5,5,5	1.05	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	M	404	-	-	4/4/4/4	-
4	EDO	K	404	-	-	1/1/1/1	-
5	N2P	F	402	-	-	1/4/4/4	-
2	GOL	B	402	-	-	2/4/4/4	-
2	GOL	F	401	-	-	2/4/4/4	-
3	PEG	L	402	-	-	0/4/4/4	-
2	GOL	K	402	-	-	2/4/4/4	-
2	GOL	O	402	-	-	2/4/4/4	-
5	N2P	L	401	-	-	1/4/4/4	-
2	GOL	F	403	-	-	2/4/4/4	-
2	GOL	D	402	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	M	402	-	-	2/4/4/4	-
4	EDO	I	404	-	-	1/1/1/1	-
2	GOL	I	401	-	-	2/4/4/4	-
2	GOL	G	403	-	-	1/4/4/4	-
2	GOL	I	403	-	-	2/4/4/4	-
2	GOL	C	402	-	-	2/4/4/4	-
4	EDO	N	403	-	-	1/1/1/1	-
2	GOL	C	403	-	-	2/4/4/4	-
5	N2P	G	401	-	-	1/4/4/4	-
4	EDO	L	403	-	-	1/1/1/1	-
4	EDO	D	403	-	-	0/1/1/1	-
2	GOL	H	401	-	-	3/4/4/4	-
5	N2P	J	401	-	-	0/4/4/4	-
5	N2P	C	401	-	-	0/4/4/4	-
4	EDO	J	402	-	-	1/1/1/1	-
5	N2P	B	401	-	-	0/4/4/4	-
5	N2P	E	401	-	-	0/4/4/4	-
2	GOL	E	402	-	-	4/4/4/4	-
3	PEG	G	402	-	-	2/4/4/4	-
2	GOL	E	403	-	-	2/4/4/4	-
2	GOL	I	402	-	-	0/4/4/4	-
2	GOL	N	402	-	-	2/4/4/4	-
6	PGE	B	403	-	-	4/7/7/7	-
4	EDO	F	404	-	-	1/1/1/1	-
5	N2P	N	401	-	-	0/4/4/4	-
4	EDO	A	405	-	-	1/1/1/1	-
5	N2P	K	401	-	-	0/4/4/4	-
2	GOL	K	403	-	-	2/4/4/4	-
2	GOL	C	404	-	-	4/4/4/4	-
2	GOL	A	404	-	-	2/4/4/4	-
2	GOL	A	402	-	-	2/4/4/4	-
4	EDO	C	405	-	-	1/1/1/1	-
2	GOL	M	403	-	-	4/4/4/4	-
2	GOL	A	401	-	-	2/4/4/4	-
5	N2P	D	401	-	-	0/4/4/4	-
5	N2P	O	401	-	-	1/4/4/4	-
2	GOL	O	403	-	-	0/4/4/4	-
3	PEG	A	403	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	N2P	M	401	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 75 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	402	GOL	O1-C1-C2-O2
2	A	404	GOL	O2-C2-C3-O3
2	B	402	GOL	C1-C2-C3-O3
2	C	404	GOL	O1-C1-C2-O2
2	C	404	GOL	O1-C1-C2-C3

There are no ring outliers.

14 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	402	N2P	3	0
2	B	402	GOL	1	0
2	F	401	GOL	1	0
5	L	401	N2P	3	0
5	G	401	N2P	2	0
5	J	401	N2P	3	0
5	C	401	N2P	3	0
5	B	401	N2P	3	0
5	E	401	N2P	3	0
5	N	401	N2P	3	0
5	K	401	N2P	3	0
5	D	401	N2P	3	0
5	O	401	N2P	3	0
5	M	401	N2P	2	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, 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	296/304 (97%)	0.38	20 (6%)	23 20	26, 55, 98, 126	3 (1%)
1	B	297/304 (97%)	-0.28	4 (1%)	75 73	29, 41, 61, 93	0
1	C	301/304 (99%)	-0.38	3 (0%)	79 77	25, 40, 57, 109	1 (0%)
1	D	298/304 (98%)	-0.47	1 (0%)	90 88	20, 37, 49, 85	3 (1%)
1	E	297/304 (97%)	-0.37	1 (0%)	90 88	29, 41, 56, 83	0
1	F	298/304 (98%)	-0.02	2 (0%)	84 82	30, 51, 71, 92	0
1	G	295/304 (97%)	1.26	54 (18%)	3 2	52, 76, 101, 114	0
1	H	268/304 (88%)	2.09	131 (48%)	0 0	59, 97, 136, 155	0
1	I	292/304 (96%)	0.22	13 (4%)	38 35	24, 49, 101, 126	1 (0%)
1	J	298/304 (98%)	-0.30	3 (1%)	79 77	27, 41, 59, 113	1 (0%)
1	K	301/304 (99%)	-0.29	3 (0%)	79 77	28, 42, 60, 116	0
1	L	298/304 (98%)	-0.47	1 (0%)	90 88	27, 38, 52, 100	2 (0%)
1	M	298/304 (98%)	-0.42	2 (0%)	84 82	28, 38, 54, 92	0
1	N	298/304 (98%)	-0.31	2 (0%)	84 82	27, 40, 55, 92	1 (0%)
1	O	298/304 (98%)	0.05	5 (1%)	69 66	34, 52, 73, 121	1 (0%)
1	P	279/304 (91%)	0.72	28 (10%)	12 10	33, 69, 116, 140	1 (0%)
All	All	4712/4864 (96%)	0.07	273 (5%)	29 25	20, 46, 98, 155	14 (0%)

The worst 5 of 273 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	193	ILE	6.2
1	A	129	GLY	6.2
1	H	185	GLY	6.1
1	H	234	ILE	6.0
1	H	135	TYR	5.6

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PEG	A	403	7/7	0.66	0.22	81,85,92,92	0
3	PEG	G	402	7/7	0.77	0.18	72,76,84,86	0
2	GOL	H	401	6/6	0.79	0.25	94,97,99,101	0
3	PEG	L	402	7/7	0.79	0.22	75,83,90,90	0
2	GOL	A	404	6/6	0.84	0.14	69,74,76,77	0
4	EDO	A	405	4/4	0.84	0.20	60,60,61,62	0
2	GOL	I	403	6/6	0.85	0.17	69,74,82,84	0
4	EDO	D	403	4/4	0.85	0.16	74,75,78,79	0
6	PGE	B	403	10/10	0.85	0.18	63,78,88,94	0
2	GOL	B	402	6/6	0.86	0.17	62,68,71,78	0
2	GOL	O	403	6/6	0.86	0.15	66,71,75,75	0
4	EDO	C	405	4/4	0.86	0.21	68,68,72,73	0
2	GOL	F	403	6/6	0.86	0.15	67,80,81,83	0
4	EDO	I	404	4/4	0.86	0.19	64,64,65,69	0
4	EDO	L	403	4/4	0.86	0.20	59,61,61,66	0
2	GOL	A	401	6/6	0.86	0.18	80,83,85,86	0
4	EDO	F	404	4/4	0.88	0.21	74,77,77,78	0
2	GOL	C	404	6/6	0.88	0.18	72,78,80,81	0
5	N2P	M	401	7/7	0.89	0.15	39,40,41,43	0
4	EDO	J	402	4/4	0.90	0.14	68,68,69,70	0
2	GOL	M	403	6/6	0.90	0.14	54,60,61,62	0
4	EDO	K	404	4/4	0.91	0.16	65,66,70,74	0
2	GOL	E	403	6/6	0.91	0.11	54,59,61,63	0
4	EDO	N	403	4/4	0.91	0.19	73,74,75,75	0
2	GOL	N	402	6/6	0.91	0.12	54,65,68,68	0
2	GOL	E	402	6/6	0.91	0.17	70,78,83,89	0
2	GOL	M	404	6/6	0.92	0.13	59,65,67,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	F	401	6/6	0.92	0.13	56,63,66,66	0
2	GOL	O	402	6/6	0.92	0.11	62,63,63,64	0
2	GOL	I	402	6/6	0.92	0.11	58,64,67,69	0
5	N2P	E	401	7/7	0.92	0.14	42,42,43,44	0
2	GOL	C	403	6/6	0.92	0.10	58,66,71,71	0
5	N2P	N	401	7/7	0.92	0.13	45,45,46,46	0
2	GOL	G	403	6/6	0.92	0.10	60,64,66,67	0
5	N2P	C	401	7/7	0.93	0.14	41,41,43,43	0
2	GOL	M	402	6/6	0.93	0.12	54,59,64,67	0
5	N2P	J	401	7/7	0.93	0.13	45,46,47,48	0
5	N2P	K	401	7/7	0.93	0.13	45,45,47,48	0
2	GOL	A	402	6/6	0.93	0.14	58,62,68,72	0
2	GOL	D	402	6/6	0.93	0.13	55,57,62,65	0
5	N2P	B	401	7/7	0.93	0.11	42,42,43,44	0
2	GOL	K	403	6/6	0.94	0.11	53,58,61,61	0
5	N2P	F	402	7/7	0.94	0.13	61,61,63,63	0
5	N2P	G	401	7/7	0.94	0.14	71,73,74,75	0
5	N2P	O	401	7/7	0.94	0.11	50,50,51,52	0
5	N2P	D	401	7/7	0.94	0.14	42,43,44,44	0
2	GOL	C	402	6/6	0.95	0.10	52,57,64,67	0
2	GOL	I	401	6/6	0.95	0.10	49,53,57,60	0
2	GOL	K	402	6/6	0.95	0.10	59,66,69,72	0
5	N2P	L	401	7/7	0.95	0.13	42,42,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.