



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 25, 2026 – 07:21 AM UTC

PDB ID : 5H8I / pdb_00005h8i
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

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:

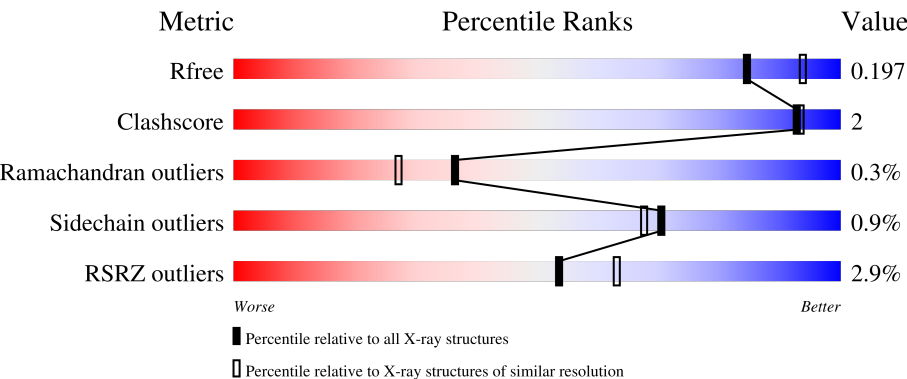
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance 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}	180053	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	5% 90% 7% .
1	B	304	% 93% 5% .
1	C	304	% 93% 5% ..
1	D	304	94% ..
1	E	304	96% ..

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Mol	Chain	Length	Quality of chain
1	F	304	% 94% • •
1	G	304	5% 90% 7% •
1	H	304	20% 83% 9% • 7%
1	I	304	3% 91% 5% •
1	J	304	% 94% • •
1	K	304	% 95% • •
1	L	304	96% • •
1	M	304	93% • •
1	N	304	93% 5% •
1	O	304	% 96% • •
1	P	304	6% 88% 6% • 5%

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:

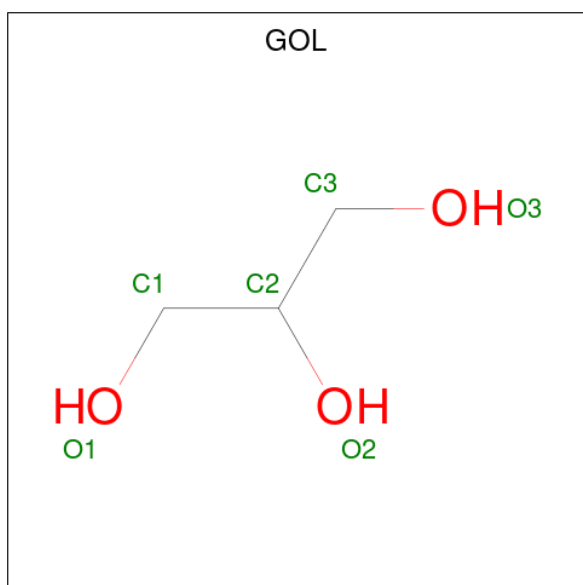
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP G7ITU5
A	-1	ASN	-	expression tag	UNP G7ITU5
A	0	ALA	-	expression tag	UNP G7ITU5
B	-2	SER	-	expression tag	UNP G7ITU5
B	-1	ASN	-	expression tag	UNP G7ITU5
B	0	ALA	-	expression tag	UNP G7ITU5
C	-2	SER	-	expression tag	UNP G7ITU5
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 (CCD ID: 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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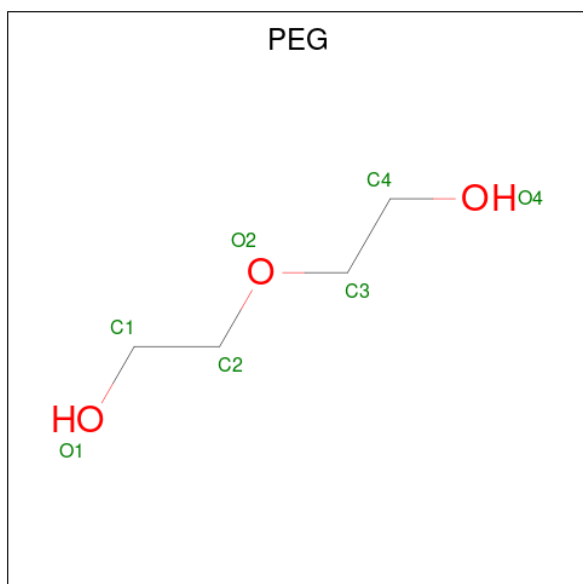
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	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 (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



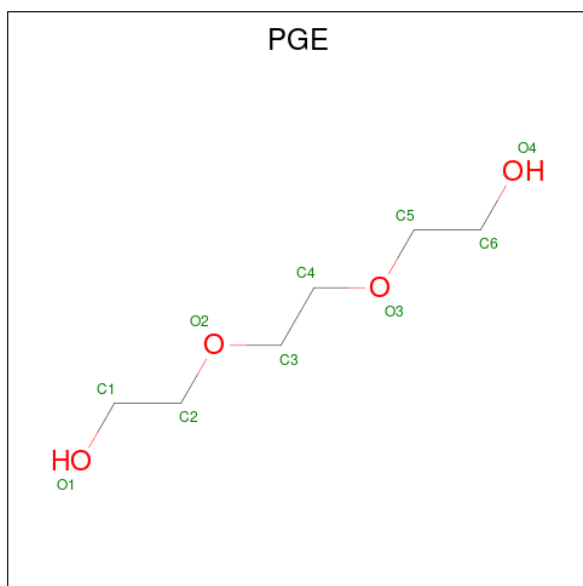
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	D	1	Total	C	O	0	0
			7	4	3		
3	D	1	Total	C	O	0	0
			7	4	3		
3	G	1	Total	C	O	0	0
			7	4	3		
3	J	1	Total	C	O	0	0
			7	4	3		

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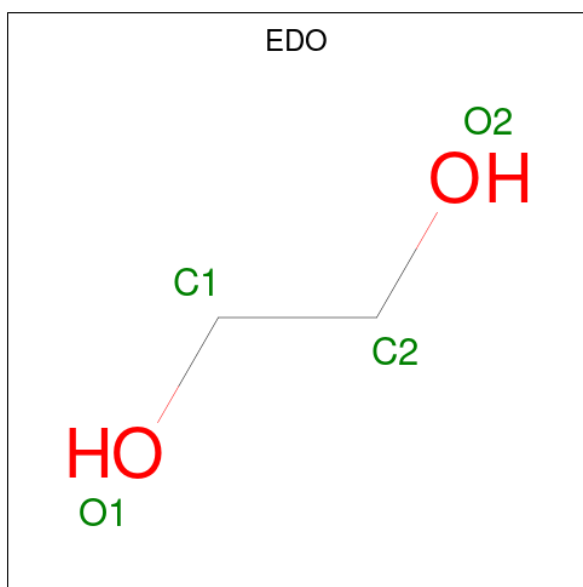
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	L	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



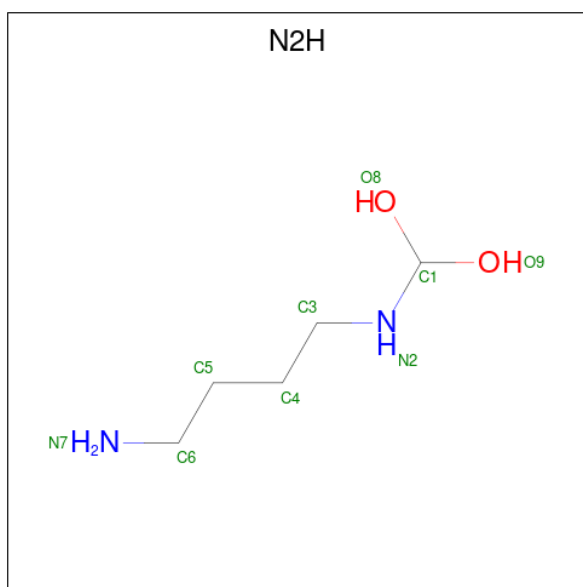
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		
4	C	1	Total	C	O	0	0
			10	6	4		
4	G	1	Total	C	O	0	0
			10	6	4		
4	J	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: 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-azanylbutoylamino)methanediol (CCD ID: N2H) (formula: $C_5H_{14}N_2O_2$).



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 (CCD ID: NA) (formula: Na).

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

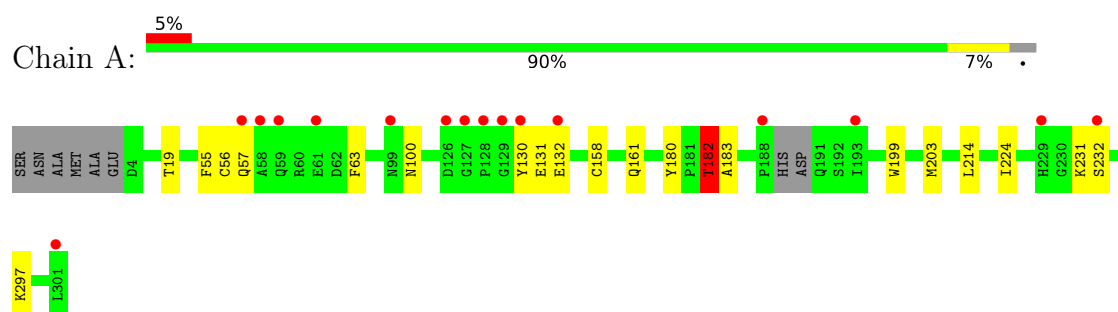
- Molecule 8 is water.

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

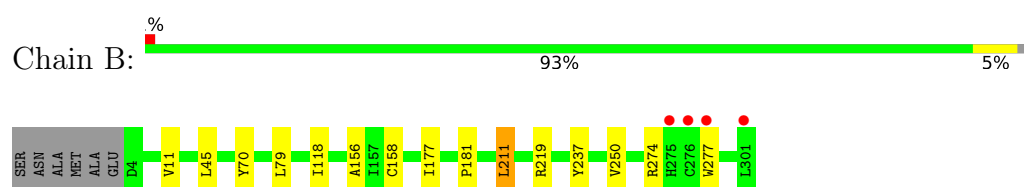
3 Residue-property plots [i](#)

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.

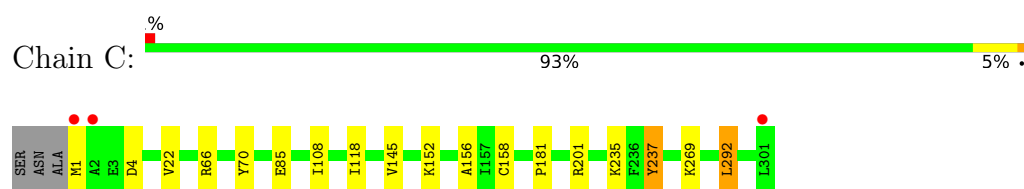
- Molecule 1: N-carbamoylputrescine amidohydrolase



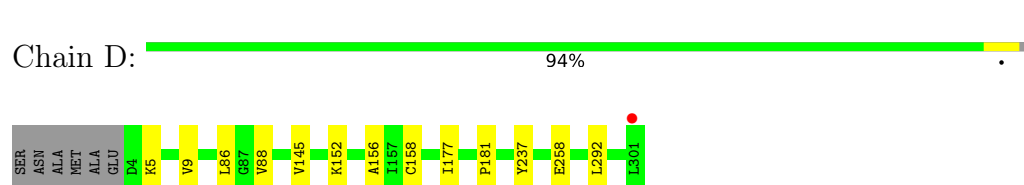
- Molecule 1: N-carbamoylputrescine amidohydrolase



- Molecule 1: N-carbamoylputrescine amidohydrolase



- Molecule 1: N-carbamoylputrescine amidohydrolase



- Molecule 1: N-carbamoylputrescine amidohydrolase

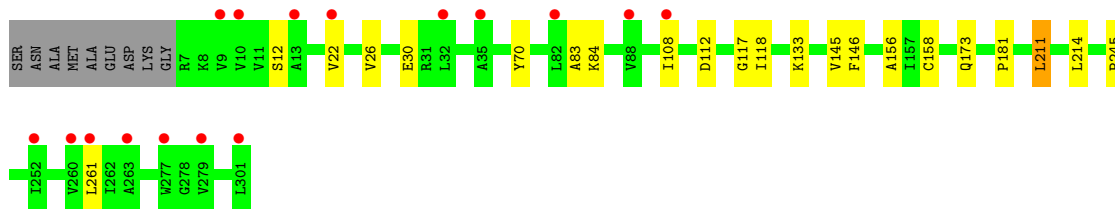
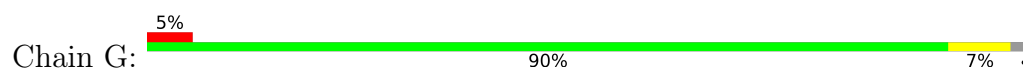




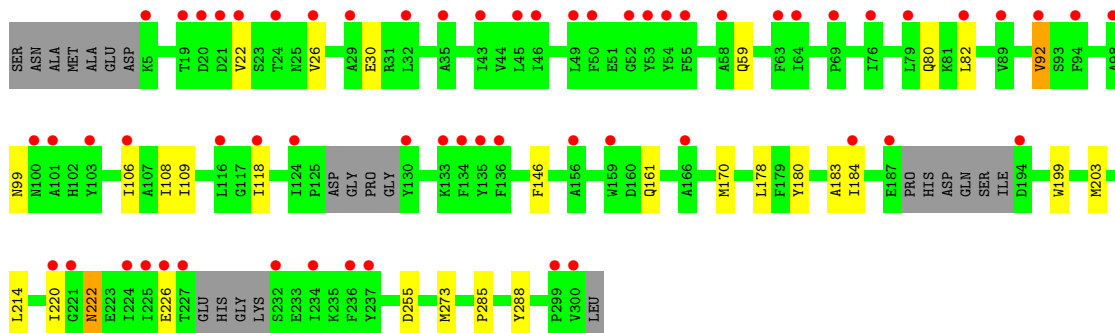
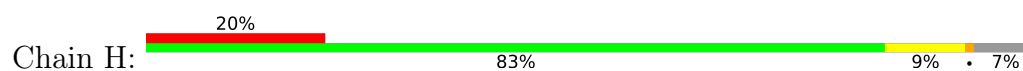
- Molecule 1: N-carbamoylputrescine amidohydrolase



- Molecule 1: N-carbamoylputrescine amidohydrolase



- Molecule 1: N-carbamoylputrescine amidohydrolase



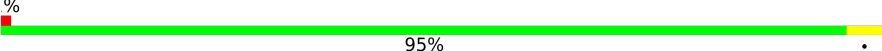
- Molecule 1: N-carbamoylputrescine amidohydrolase



- Molecule 1: N-carbamoylputrescine amidohydrolase

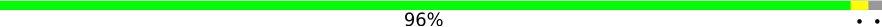


- Molecule 1: N-carbamoylputrescine amidohydrolase

Chain K:  95%



- Molecule 1: N-carbamoylputrescine amidohydrolase

Chain L:  96%



- Molecule 1: N-carbamoylputrescine amidohydrolase

Chain M:  93%

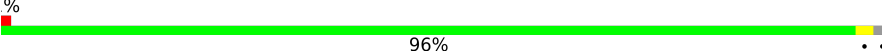


- Molecule 1: N-carbamoylputrescine amidohydrolase

Chain N:  93% 5%



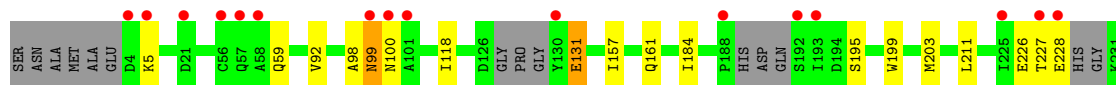
- Molecule 1: N-carbamoylputrescine amidohydrolase

Chain O:  96%



- Molecule 1: N-carbamoylputrescine amidohydrolase

Chain P:  88% 6% 6% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	26.3	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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 ²)	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.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, N2H, PGE, 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	1.01	0/2422	0.95	4/3274 (0.1%)
1	B	1.02	1/2435 (0.0%)	0.92	2/3295 (0.1%)
1	C	1.04	1/2470 (0.0%)	0.92	1/3342 (0.0%)
1	D	1.04	0/2455	0.91	0/3323
1	E	1.01	0/2435	0.92	1/3295 (0.0%)
1	F	0.98	2/2449 (0.1%)	0.94	2/3314 (0.1%)
1	G	1.09	1/2407 (0.0%)	0.93	2/3258 (0.1%)
1	H	1.07	0/2308	0.94	2/3117 (0.1%)
1	I	1.01	1/2384 (0.0%)	0.93	4/3223 (0.1%)
1	J	1.00	0/2448	0.93	1/3313 (0.0%)
1	K	1.00	2/2477 (0.1%)	0.91	0/3352
1	L	1.02	0/2448	0.90	0/3313
1	M	1.04	5/2447 (0.2%)	0.92	0/3312
1	N	1.01	0/2449	0.91	1/3314 (0.0%)
1	O	1.01	0/2429	0.89	0/3286
1	P	0.93	0/2360	0.89	2/3188 (0.1%)
All	All	1.02	13/38823 (0.0%)	0.92	22/52519 (0.0%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	297	LYS	C-O	-6.07	1.16	1.24
1	K	149	LYS	C-O	-5.58	1.17	1.24
1	M	68	LYS	C-O	-5.55	1.18	1.24
1	M	149	LYS	C-O	-5.41	1.17	1.24
1	I	284	ARG	CA-C	5.37	1.59	1.53
1	F	117	GLY	C-O	5.36	1.28	1.23
1	B	250	VAL	C-O	-5.33	1.19	1.24
1	F	188	PRO	C-O	-5.31	1.17	1.24
1	M	250[A]	VAL	C-O	-5.23	1.18	1.24
1	M	250[B]	VAL	C-O	-5.23	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	85	GLU	C-O	-5.14	1.18	1.24
1	K	188	PRO	C-O	-5.09	1.17	1.24
1	G	117	GLY	C-O	5.09	1.28	1.23

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	226	GLU	N-CA-C	7.32	120.45	110.35
1	A	132	GLU	N-CA-C	6.65	119.35	111.71
1	C	237	TYR	N-CA-C	5.78	119.31	112.72
1	I	157	ILE	N-CA-C	5.67	116.28	108.12
1	I	22	VAL	N-CA-C	5.64	116.28	110.36
1	A	56	CYS	N-CA-C	5.38	119.10	112.54
1	E	237	TYR	N-CA-C	5.32	118.78	112.72
1	F	104	ASN	N-CA-C	-5.30	99.13	108.20
1	P	157	ILE	N-CA-C	5.29	115.52	108.11
1	P	92	VAL	N-CA-C	5.28	114.34	106.85
1	J	196	ARG	N-CA-C	5.26	117.02	111.28
1	F	118	ILE	N-CA-C	5.25	117.18	108.99
1	G	83	ALA	CA-C-N	5.24	127.25	120.44
1	G	83	ALA	C-N-CA	5.24	127.25	120.44
1	A	19	THR	N-CA-C	-5.13	103.16	110.59
1	B	45	LEU	N-CA-C	5.11	116.85	108.52
1	B	219	ARG	N-CA-CB	-5.10	103.07	110.36
1	H	92	VAL	N-CA-C	5.08	114.06	106.85
1	I	298	ASN	N-CA-C	5.04	116.25	109.24
1	A	182	THR	CB-CA-C	-5.02	99.47	110.67
1	N	237	TYR	N-CA-C	5.02	118.72	112.59
1	I	45	LEU	N-CA-C	5.00	116.68	108.52

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	14	0
1	B	2373	0	2340	6	0
1	C	2402	0	2377	9	0
1	D	2384	0	2363	6	0
1	E	2370	0	2340	2	0
1	F	2381	0	2349	6	0
1	G	2348	0	2311	12	0
1	H	2253	0	2231	17	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	10	0
1	O	2367	0	2333	2	0
1	P	2304	0	2277	12	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	1	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	116	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.

All (116) 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:N:245:PRO:HB2	1:N:273:MET:HE1	1.78	0.65
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:P:211:LEU:HD23	1:P:273[A]:MET:HE3	1.86	0.57
1:M:273:MET:HE1	8:M:829:HOH:O	2.03	0.56
1:N:211:LEU:HD23	1:N:273:MET:HE3	1.87	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:A:161:GLN:HB2	1:A:203[B]:MET:HE3	1.89	0.53
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: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:199:TRP:O	1:I:203:MET:HG2	2.09	0.52
1:I:273:MET:HE1	8:I:746:HOH:O	2.08	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:L:273:MET:HE1	8:L:843:HOH:O	2.10	0.50
1:N:245:PRO:CB	1:N:273:MET:HE1	2.42	0.49
1:O:45:LEU:HD11	1:O:181:PRO:HG3	1.94	0.49
1:N:245:PRO:CG	1:N:273:MET:HE1	2.42	0.49
1:H:222:ASN:N	1:H:222:ASN:OD1	2.46	0.49
1:K:145[B]:VAL:CG1	1:K:152:LYS:HG2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:F:4:ASP:O	1:F:8:LYS:NZ	2.43	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:H:180:TYR:CG	1:H:203:MET:HE1	2.50	0.46
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:HA	1:A:57:GLN:OE1	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:G:214:LEU:C	1:G:214:LEU:HD23	2.41	0.46
1:I:292:LEU:HD22	1:J:292:LEU:HD11	1.98	0.46
1:C:4:ASP:OD2	1:C:269:LYS:NZ	2.45	0.45
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: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:A:180:TYR:CD1	1:A:203[B]:MET:HE2	2.53	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:H:170:MET:HE3	1:H:178:LEU:HD22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:H:92:VAL:C	1:H:106:ILE:HG13	2.45	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:E:273:MET:HE1	8:E:835:HOH:O	2.20	0.41
1:I:161:GLN:HB2	1:I:203:MET:SD	2.61	0.41
1:A:214:LEU:HD23	1:A:214:LEU:C	2.45	0.41
1:H:220:ILE:HD11	1:H:255:ASP:C	2.45	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: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:HD23	1:B:79:LEU:HA	1.93	0.41
1:G:26:VAL:O	1:G:30:GLU:HG3	2.21	0.41
1:H:214:LEU:C	1:H:214:LEU:HD23	2.46	0.40
1:K:145[B]:VAL:CG1	1:K:152:LYS:CG	2.99	0.40
1:A:203[B]:MET:HE1	8:A:502:HOH:O	2.21	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

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	295/304 (97%)	282 (96%)	13 (4%)	0	100	100
1	B	298/304 (98%)	287 (96%)	10 (3%)	1 (0%)	36	27
1	C	303/304 (100%)	294 (97%)	8 (3%)	1 (0%)	36	27
1	D	301/304 (99%)	294 (98%)	6 (2%)	1 (0%)	36	27
1	E	298/304 (98%)	287 (96%)	10 (3%)	1 (0%)	36	27
1	F	300/304 (99%)	287 (96%)	12 (4%)	1 (0%)	36	27
1	G	294/304 (97%)	283 (96%)	10 (3%)	1 (0%)	36	27
1	H	276/304 (91%)	265 (96%)	9 (3%)	2 (1%)	18	9
1	I	290/304 (95%)	280 (97%)	10 (3%)	0	100	100
1	J	300/304 (99%)	292 (97%)	7 (2%)	1 (0%)	36	27
1	K	304/304 (100%)	293 (96%)	10 (3%)	1 (0%)	36	27
1	L	300/304 (99%)	289 (96%)	10 (3%)	1 (0%)	36	27
1	M	300/304 (99%)	292 (97%)	7 (2%)	1 (0%)	36	27
1	N	300/304 (99%)	289 (96%)	10 (3%)	1 (0%)	36	27
1	O	297/304 (98%)	288 (97%)	8 (3%)	1 (0%)	36	27
1	P	283/304 (93%)	277 (98%)	6 (2%)	0	100	100
All	All	4739/4864 (97%)	4579 (97%)	146 (3%)	14 (0%)	36	27

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

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Mol	Chain	Res	Type
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%)	48	42
1	B	250/252 (99%)	248 (99%)	2 (1%)	73	71
1	C	254/252 (101%)	250 (98%)	4 (2%)	55	50
1	D	253/252 (100%)	251 (99%)	2 (1%)	73	71
1	E	250/252 (99%)	248 (99%)	2 (1%)	73	71
1	F	252/252 (100%)	252 (100%)	0	100	100
1	G	247/252 (98%)	246 (100%)	1 (0%)	84	82
1	H	237/252 (94%)	235 (99%)	2 (1%)	73	71
1	I	244/252 (97%)	240 (98%)	4 (2%)	55	50
1	J	252/252 (100%)	250 (99%)	2 (1%)	73	71
1	K	255/252 (101%)	252 (99%)	3 (1%)	63	58
1	L	252/252 (100%)	252 (100%)	0	100	100
1	M	252/252 (100%)	249 (99%)	3 (1%)	63	58
1	N	252/252 (100%)	251 (100%)	1 (0%)	84	82
1	O	249/252 (99%)	247 (99%)	2 (1%)	73	71
1	P	243/252 (96%)	239 (98%)	4 (2%)	55	50
All	All	3991/4032 (99%)	3954 (99%)	37 (1%)	70	67

All (37) 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	232	SER
1	A	297	LYS
1	B	211	LEU
1	B	237	TYR
1	C	1	MET
1	C	108	ILE
1	C	237	TYR
1	C	292	LEU
1	D	5	LYS
1	D	237	TYR
1	E	5	LYS
1	E	237	TYR
1	G	211	LEU
1	H	118	ILE
1	H	222	ASN
1	I	184	ILE
1	I	222	ASN
1	I	300	VAL
1	I	301	LEU
1	J	5	LYS
1	J	211	LEU
1	K	1	MET
1	K	5	LYS
1	K	237	TYR
1	M	5	LYS
1	M	237	TYR
1	M	301	LEU
1	N	7	ARG
1	O	5	LYS
1	O	211	LEU
1	P	99	ASN
1	P	118	ILE
1	P	131	GLU
1	P	226	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	65	GLN
1	A	204	GLN
1	B	204	GLN
1	B	229	HIS
1	B	298	ASN
1	C	298	ASN
1	D	204	GLN
1	D	298	ASN
1	E	39	GLN
1	E	298	ASN
1	F	39	GLN
1	F	59	GLN
1	F	204	GLN
1	G	37	HIS
1	G	173	GLN
1	H	39	GLN
1	H	99	ASN
1	H	161	GLN
1	H	204	GLN
1	I	39	GLN
1	I	222	ASN
1	J	204	GLN
1	K	298	ASN
1	L	204	GLN
1	L	298	ASN
1	M	204	GLN
1	M	222	ASN
1	M	298	ASN
1	O	39	GLN
1	O	59	GLN
1	O	204	GLN
1	P	37	HIS
1	P	59	GLN
1	P	99	ASN
1	P	102	HIS
1	P	161	GLN
1	P	222	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	$\# Z > 2$
6	N2H	E	401	1	8,8,8	2.24	1 (12%)	5,8,8	2.31	1 (20%)
6	N2H	G	401	1	8,8,8	2.57	2 (25%)	5,8,8	1.63	1 (20%)
2	GOL	A	402	-	5,5,5	0.43	0	5,5,5	0.46	0
2	GOL	B	402	-	5,5,5	0.15	0	5,5,5	0.61	0
6	N2H	F	401	1	8,8,8	2.37	3 (37%)	5,8,8	1.60	1 (20%)
2	GOL	J	404	-	5,5,5	0.23	0	5,5,5	0.49	0
2	GOL	J	403	-	5,5,5	0.52	0	5,5,5	0.35	0
2	GOL	K	403	-	5,5,5	0.50	0	5,5,5	0.48	0
2	GOL	C	403	-	5,5,5	0.26	0	5,5,5	0.37	0
2	GOL	N	404	-	5,5,5	0.43	0	5,5,5	0.45	0
6	N2H	L	401	1	8,8,8	2.18	2 (25%)	5,8,8	2.05	1 (20%)
2	GOL	J	405	-	5,5,5	0.72	0	5,5,5	1.20	1 (20%)
3	PEG	D	404	-	6,6,6	0.48	0	5,5,5	0.36	0
2	GOL	A	403	-	5,5,5	0.34	0	5,5,5	0.33	0
5	EDO	N	405	-	3,3,3	0.45	0	2,2,2	0.30	0
2	GOL	E	405	-	5,5,5	0.49	0	5,5,5	0.22	0
2	GOL	N	402	-	5,5,5	0.45	0	5,5,5	0.70	0
4	PGE	G	404	-	9,9,9	0.49	0	8,8,8	0.26	0
2	GOL	I	402	-	5,5,5	0.68	0	5,5,5	0.64	0
6	N2H	B	401	1	8,8,8	2.04	2 (25%)	5,8,8	1.75	1 (20%)
3	PEG	L	403	-	6,6,6	0.50	0	5,5,5	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PEG	D	405	-	6,6,6	0.47	0	5,5,5	0.64	0
5	EDO	K	405	-	3,3,3	0.54	0	2,2,2	0.16	0
2	GOL	F	403	-	5,5,5	0.63	0	5,5,5	0.86	0
2	GOL	N	403	-	5,5,5	0.36	0	5,5,5	0.21	0
2	GOL	C	405	-	5,5,5	0.33	0	5,5,5	0.46	0
2	GOL	B	403	-	5,5,5	0.38	0	5,5,5	0.51	0
2	GOL	M	403	-	5,5,5	0.40	0	5,5,5	0.17	0
2	GOL	F	402	-	5,5,5	0.35	0	5,5,5	0.18	0
6	N2H	J	401	1	8,8,8	2.65	3 (37%)	5,8,8	1.79	1 (20%)
6	N2H	O	401	1	8,8,8	2.41	1 (12%)	5,8,8	2.08	1 (20%)
2	GOL	D	402	-	5,5,5	0.42	0	5,5,5	1.21	0
2	GOL	I	401	-	5,5,5	0.45	0	5,5,5	0.26	0
2	GOL	K	404	-	5,5,5	0.19	0	5,5,5	0.26	0
2	GOL	M	402	-	5,5,5	0.28	0	5,5,5	0.57	0
4	PGE	A	405	-	9,9,9	0.54	0	8,8,8	0.46	0
2	GOL	H	401	-	5,5,5	0.39	0	5,5,5	0.83	0
3	PEG	A	404	-	6,6,6	0.51	0	5,5,5	0.18	0
2	GOL	L	402	-	5,5,5	0.30	0	5,5,5	0.24	0
4	PGE	J	407	-	9,9,9	0.57	0	8,8,8	0.34	0
5	EDO	C	407	-	3,3,3	0.58	0	2,2,2	0.10	0
6	N2H	C	401	1	8,8,8	2.10	2 (25%)	5,8,8	2.31	1 (20%)
5	EDO	A	406	-	3,3,3	0.50	0	2,2,2	0.33	0
6	N2H	K	401	1	8,8,8	2.37	3 (37%)	5,8,8	2.20	1 (20%)
3	PEG	J	406	-	6,6,6	0.52	0	5,5,5	0.27	0
6	N2H	N	401	1	8,8,8	2.35	2 (25%)	5,8,8	2.13	1 (20%)
6	N2H	M	401	1	8,8,8	2.16	2 (25%)	5,8,8	2.40	1 (20%)
2	GOL	A	401	-	5,5,5	0.40	0	5,5,5	0.26	0
2	GOL	O	402	-	5,5,5	0.11	0	5,5,5	0.60	0
6	N2H	D	401	1	8,8,8	2.39	2 (25%)	5,8,8	2.21	1 (20%)
2	GOL	E	404	-	5,5,5	0.32	0	5,5,5	0.41	0
3	PEG	G	403	-	6,6,6	0.51	0	5,5,5	0.21	0
2	GOL	E	402	-	5,5,5	0.45	0	5,5,5	0.38	0
2	GOL	K	402	-	5,5,5	0.27	0	5,5,5	0.65	0
5	EDO	P	401	-	3,3,3	0.54	0	2,2,2	0.21	0
2	GOL	D	403	-	5,5,5	0.40	0	5,5,5	0.43	0
2	GOL	C	404	-	5,5,5	0.36	0	5,5,5	0.40	0
5	EDO	D	406	-	3,3,3	0.51	0	2,2,2	0.17	0
2	GOL	G	402	-	5,5,5	0.39	0	5,5,5	0.27	0
4	PGE	C	406	-	9,9,9	0.55	0	8,8,8	0.25	0
2	GOL	J	402	-	5,5,5	0.31	0	5,5,5	0.33	0
2	GOL	C	402	-	5,5,5	0.67	0	5,5,5	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	E	403	-	5,5,5	0.50	0	5,5,5	0.17	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
6	N2H	E	401	1	-	0/4/6/6	-
6	N2H	G	401	1	-	0/4/6/6	-
2	GOL	A	402	-	-	0/4/4/4	-
2	GOL	B	402	-	-	4/4/4/4	-
6	N2H	F	401	1	-	0/4/6/6	-
2	GOL	J	404	-	-	2/4/4/4	-
2	GOL	J	403	-	-	4/4/4/4	-
2	GOL	K	403	-	-	4/4/4/4	-
2	GOL	C	403	-	-	0/4/4/4	-
2	GOL	N	404	-	-	0/4/4/4	-
6	N2H	L	401	1	-	1/4/6/6	-
2	GOL	J	405	-	-	2/4/4/4	-
3	PEG	D	404	-	-	2/4/4/4	-
2	GOL	A	403	-	-	1/4/4/4	-
5	EDO	N	405	-	-	1/1/1/1	-
2	GOL	E	405	-	-	0/4/4/4	-
2	GOL	N	402	-	-	4/4/4/4	-
4	PGE	G	404	-	-	1/7/7/7	-
2	GOL	I	402	-	-	3/4/4/4	-
6	N2H	B	401	1	-	0/4/6/6	-
3	PEG	L	403	-	-	2/4/4/4	-
3	PEG	D	405	-	-	3/4/4/4	-
5	EDO	K	405	-	-	1/1/1/1	-
2	GOL	F	403	-	-	2/4/4/4	-
2	GOL	N	403	-	-	0/4/4/4	-
2	GOL	C	405	-	-	2/4/4/4	-
2	GOL	B	403	-	-	1/4/4/4	-
2	GOL	M	403	-	-	4/4/4/4	-
2	GOL	F	402	-	-	2/4/4/4	-
6	N2H	J	401	1	-	0/4/6/6	-
6	N2H	O	401	1	-	0/4/6/6	-

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

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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	3.27	1.53	1.47
6	J	401	N2H	O8-C1	3.23	1.48	1.40
6	J	401	N2H	C3-N2	3.16	1.53	1.47
6	M	401	N2H	O8-C1	2.71	1.46	1.40
6	B	401	N2H	O8-C1	2.65	1.46	1.40
6	F	401	N2H	C3-N2	2.60	1.52	1.47
6	K	401	N2H	C3-N2	2.55	1.52	1.47
6	C	401	N2H	C3-N2	2.48	1.52	1.47
6	L	401	N2H	O8-C1	2.44	1.46	1.40
6	D	401	N2H	O8-C1	2.32	1.45	1.40
6	F	401	N2H	O9-C1	2.23	1.45	1.40
6	N	401	N2H	C3-N2	2.16	1.51	1.47
6	K	401	N2H	O8-C1	2.10	1.45	1.40

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	401	N2H	O8-C1-O9	-5.15	100.85	111.31
6	E	401	N2H	O8-C1-O9	-4.87	101.43	111.31
6	C	401	N2H	O8-C1-O9	-4.73	101.70	111.31
6	D	401	N2H	O8-C1-O9	-4.48	102.21	111.31
6	N	401	N2H	O8-C1-O9	-4.44	102.29	111.31
6	K	401	N2H	O8-C1-O9	-4.44	102.30	111.31
6	O	401	N2H	O8-C1-O9	-4.43	102.32	111.31
6	L	401	N2H	O8-C1-O9	-4.18	102.82	111.31
6	J	401	N2H	O8-C1-O9	-3.65	103.89	111.31
6	B	401	N2H	O8-C1-O9	-3.55	104.11	111.31
6	F	401	N2H	O8-C1-O9	-3.25	104.71	111.31
6	G	401	N2H	O8-C1-O9	-3.22	104.76	111.31
2	J	405	GOL	O3-C3-C2	2.22	120.35	110.38

There are no chirality outliers.

All (91) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
4	C	406	PGE	O3-C5-C6-O4
2	B	402	GOL	O1-C1-C2-O2
2	B	402	GOL	O2-C2-C3-O3
2	E	402	GOL	O2-C2-C3-O3
2	E	403	GOL	O2-C2-C3-O3
2	F	403	GOL	O2-C2-C3-O3
2	G	402	GOL	O1-C1-C2-O2
2	J	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	N	402	GOL	O1-C1-C2-O2
2	N	402	GOL	O2-C2-C3-O3
2	O	402	GOL	O2-C2-C3-O3
3	J	406	PEG	O1-C1-C2-O2
3	J	406	PEG	O2-C3-C4-O4
5	A	406	EDO	O1-C1-C2-O2
5	D	406	EDO	O1-C1-C2-O2
5	N	405	EDO	O1-C1-C2-O2
5	C	407	EDO	O1-C1-C2-O2
5	P	401	EDO	O1-C1-C2-O2
2	J	402	GOL	O1-C1-C2-O2
2	M	403	GOL	O2-C2-C3-O3
3	L	403	PEG	O2-C3-C4-O4
4	J	407	PGE	C1-C2-O2-C3
2	A	403	GOL	O1-C1-C2-C3
2	M	402	GOL	C1-C2-C3-O3
3	D	405	PEG	C4-C3-O2-C2
3	L	403	PEG	O1-C1-C2-O2
5	K	405	EDO	O1-C1-C2-O2
4	J	407	PGE	O1-C1-C2-O2
4	C	406	PGE	C1-C2-O2-C3
3	A	404	PEG	O2-C3-C4-O4
4	J	407	PGE	C3-C4-O3-C5
6	L	401	N2H	N2-C3-C4-C5
3	D	405	PEG	O2-C3-C4-O4
2	M	403	GOL	O1-C1-C2-O2
4	A	405	PGE	C4-C3-O2-C2
2	B	403	GOL	O2-C2-C3-O3
2	F	402	GOL	O1-C1-C2-O2
2	K	403	GOL	O1-C1-C2-O2
3	D	405	PEG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	D	404	PEG	C4-C3-O2-C2
3	J	406	PEG	C4-C3-O2-C2
3	G	403	PEG	C4-C3-O2-C2
3	D	404	PEG	O1-C1-C2-O2
2	I	402	GOL	O1-C1-C2-O2
3	G	403	PEG	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 7 short contacts:

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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%)	-0.00	16 (5%)	31 40	15, 32, 76, 95	3 (1%)
1	B	298/304 (98%)	-0.45	4 (1%)	75 82	16, 26, 43, 85	2 (0%)
1	C	301/304 (99%)	-0.58	3 (0%)	79 86	14, 25, 38, 82	4 (1%)
1	D	298/304 (98%)	-0.59	1 (0%)	90 93	13, 24, 36, 71	5 (1%)
1	E	297/304 (97%)	-0.59	1 (0%)	90 93	15, 26, 38, 66	3 (1%)
1	F	298/304 (98%)	-0.42	3 (1%)	79 86	15, 29, 43, 79	4 (1%)
1	G	295/304 (97%)	0.58	16 (5%)	31 40	27, 42, 58, 70	1 (0%)
1	H	282/304 (92%)	1.25	60 (21%)	2 3	24, 57, 91, 106	2 (0%)
1	I	293/304 (96%)	-0.12	8 (2%)	56 66	17, 30, 69, 113	1 (0%)
1	J	298/304 (98%)	-0.47	2 (0%)	84 89	15, 26, 40, 96	4 (1%)
1	K	301/304 (99%)	-0.52	3 (0%)	79 86	14, 27, 41, 86	5 (1%)
1	L	298/304 (98%)	-0.63	1 (0%)	90 93	16, 23, 36, 76	4 (1%)
1	M	297/304 (97%)	-0.64	1 (0%)	90 93	16, 24, 36, 59	5 (1%)
1	N	298/304 (98%)	-0.57	1 (0%)	90 93	16, 24, 37, 69	4 (1%)
1	O	297/304 (97%)	-0.13	2 (0%)	84 89	21, 35, 50, 78	2 (0%)
1	P	289/304 (95%)	0.39	17 (5%)	28 37	20, 47, 87, 100	2 (0%)
All	All	4736/4864 (97%)	-0.23	139 (2%)	53 63	13, 29, 63, 113	51 (1%)

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	193	ILE	6.1
1	H	224	ILE	5.9
1	A	130	TYR	5.6
1	H	225	ILE	5.2
1	A	128	PRO	5.2

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Mol	Chain	Res	Type	RSRZ
1	H	130	TYR	4.8
1	H	227	THR	4.6
1	P	188	PRO	4.6
1	I	301	LEU	4.5
1	I	128	PRO	4.3
1	A	301	LEU	4.2
1	P	130	TYR	4.1
1	H	19	THR	4.1
1	H	300	VAL	4.0
1	H	58	ALA	3.9
1	P	58	ALA	3.9
1	H	234	ILE	3.8
1	I	130	TYR	3.8
1	H	134	PHE	3.6
1	O	301	LEU	3.6
1	A	129	GLY	3.6
1	P	193	ILE	3.6
1	H	101	ALA	3.5
1	H	69	PRO	3.5
1	H	76	ILE	3.5
1	B	277	TRP	3.4
1	H	64	ILE	3.4
1	I	229	HIS	3.3
1	I	230	GLY	3.3
1	H	159	TRP	3.3
1	C	301	LEU	3.3
1	B	301	LEU	3.2
1	H	63	PHE	3.2
1	I	300	VAL	3.2
1	P	300	VAL	3.2
1	A	127	GLY	3.2
1	A	126	ASP	3.2
1	P	228	GLU	3.2
1	F	301	LEU	3.1
1	C	2	ALA	3.1
1	H	22	VAL	3.1
1	H	24	THR	3.0
1	M	301	LEU	3.0
1	G	10	VAL	3.0
1	H	54	TYR	3.0
1	I	129	GLY	3.0
1	G	260	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	H	53	TYR	2.9
1	H	50	PHE	2.9
1	H	55	PHE	2.9
1	H	236	PHE	2.9
1	H	98	ALA	2.9
1	H	46	ILE	2.9
1	H	92	VAL	2.9
1	H	79	LEU	2.9
1	P	5	LYS	2.8
1	E	301	LEU	2.8
1	J	301	LEU	2.8
1	P	227	THR	2.8
1	K	301	LEU	2.8
1	H	26	VAL	2.8
1	G	82	LEU	2.8
1	G	301	LEU	2.8
1	H	49	LEU	2.8
1	A	59	GLN	2.7
1	D	301	LEU	2.7
1	G	252	ILE	2.7
1	H	20	ASP	2.6
1	B	275	HIS	2.6
1	G	261	LEU	2.6
1	H	184	ILE	2.6
1	H	35	ALA	2.6
1	G	22	VAL	2.6
1	A	188	PRO	2.5
1	G	32	LEU	2.5
1	G	35	ALA	2.5
1	G	9	VAL	2.5
1	H	82	LEU	2.5
1	G	263	ALA	2.5
1	P	4	ASP	2.5
1	H	5	LYS	2.4
1	K	2	ALA	2.4
1	H	94	PHE	2.4
1	H	133	LYS	2.4
1	H	232	SER	2.4
1	O	276	CYS	2.4
1	P	56	CYS	2.4
1	H	116	LEU	2.4
1	H	52	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	226	GLU	2.3
1	H	29	ALA	2.3
1	H	118	ILE	2.3
1	P	101	ALA	2.3
1	F	4	ASP	2.3
1	A	57	GLN	2.3
1	H	103	TYR	2.3
1	G	279	VAL	2.3
1	P	21	ASP	2.3
1	A	58	ALA	2.3
1	A	232	SER	2.3
1	H	21	ASP	2.3
1	P	99	ASN	2.3
1	H	156	ALA	2.2
1	H	106	ILE	2.2
1	H	45	LEU	2.2
1	N	228	GLU	2.2
1	H	220	ILE	2.2
1	H	89	VAL	2.2
1	P	57	GLN	2.2
1	I	127	GLY	2.2
1	C	1	MET	2.2
1	J	277	TRP	2.2
1	H	100	ASN	2.2
1	H	187	GLU	2.2
1	H	299	PRO	2.2
1	H	166	ALA	2.2
1	A	229	HIS	2.1
1	H	135	TYR	2.1
1	H	124	ILE	2.1
1	H	221	GLY	2.1
1	L	301	LEU	2.1
1	P	100	ASN	2.1
1	P	225	ILE	2.1
1	K	1	MET	2.1
1	H	32	LEU	2.1
1	H	43	ILE	2.1
1	A	99	ASN	2.1
1	G	88	VAL	2.1
1	F	191	GLN	2.1
1	B	276	CYS	2.1
1	A	132	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	108	ILE	2.0
1	G	277	TRP	2.0
1	G	13	ALA	2.0
1	H	194	ASP	2.0
1	A	61	GLU	2.0
1	P	192	SER	2.0
1	H	136	PHE	2.0
1	H	237	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	PGE	G	404	10/10	0.54	0.24	64,88,100,103	0
2	GOL	A	402	6/6	0.66	0.16	56,59,61,61	0
3	PEG	G	403	7/7	0.70	0.18	66,70,73,74	0
3	PEG	D	405	7/7	0.77	0.21	63,63,70,71	0
4	PGE	A	405	10/10	0.81	0.17	46,61,66,68	0
3	PEG	J	406	7/7	0.83	0.16	68,70,72,72	0
2	GOL	J	404	6/6	0.83	0.17	53,59,61,61	0
2	GOL	N	404	6/6	0.83	0.13	55,56,59,60	0
5	EDO	K	405	4/4	0.84	0.17	44,50,51,56	0
2	GOL	B	403	6/6	0.85	0.16	46,56,58,59	0
3	PEG	A	404	7/7	0.85	0.16	68,69,71,71	0
6	N2H	O	401	9/9	0.85	0.17	41,43,45,51	0
4	PGE	J	407	10/10	0.86	0.15	50,68,73,75	0
5	EDO	C	407	4/4	0.86	0.16	44,47,48,50	0
4	PGE	C	406	10/10	0.86	0.16	59,61,64,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	P	401	4/4	0.86	0.17	49,51,52,54	0
6	N2H	G	401	9/9	0.86	0.14	44,45,45,46	0
2	GOL	I	402	6/6	0.86	0.16	36,44,45,46	0
5	EDO	N	405	4/4	0.87	0.17	52,53,54,54	0
6	N2H	M	401	9/9	0.87	0.14	24,27,35,37	0
5	EDO	A	406	4/4	0.87	0.16	50,50,51,52	0
2	GOL	A	403	6/6	0.88	0.14	59,64,67,68	0
2	GOL	A	401	6/6	0.88	0.12	50,54,59,60	0
6	N2H	B	401	9/9	0.88	0.13	30,33,37,37	0
6	N2H	E	401	9/9	0.88	0.13	31,32,36,38	0
2	GOL	C	404	6/6	0.88	0.14	48,56,59,60	0
6	N2H	J	401	9/9	0.88	0.12	29,33,35,36	0
2	GOL	F	403	6/6	0.88	0.15	36,46,48,48	0
3	PEG	D	404	7/7	0.88	0.14	58,60,61,61	0
2	GOL	E	405	6/6	0.89	0.11	59,64,66,66	0
2	GOL	J	403	6/6	0.89	0.12	43,49,51,52	0
6	N2H	C	401	9/9	0.89	0.12	28,30,36,38	0
2	GOL	G	402	6/6	0.89	0.11	43,47,50,50	0
6	N2H	F	401	9/9	0.89	0.14	39,40,41,45	0
2	GOL	J	405	6/6	0.89	0.14	29,33,38,39	6
5	EDO	D	406	4/4	0.89	0.18	53,54,55,55	0
6	N2H	K	401	9/9	0.89	0.14	31,32,39,41	0
6	N2H	L	401	9/9	0.89	0.12	28,32,36,38	0
2	GOL	H	401	6/6	0.89	0.14	57,61,62,63	0
2	GOL	I	401	6/6	0.89	0.11	44,45,48,50	0
2	GOL	E	403	6/6	0.90	0.15	49,58,64,71	0
2	GOL	E	404	6/6	0.90	0.12	34,41,42,45	0
2	GOL	C	405	6/6	0.90	0.11	37,50,54,54	0
2	GOL	K	404	6/6	0.90	0.10	41,46,50,54	0
6	N2H	N	401	9/9	0.90	0.12	33,35,38,42	0
2	GOL	E	402	6/6	0.90	0.13	40,50,54,58	0
2	GOL	C	403	6/6	0.91	0.10	35,44,48,53	0
3	PEG	L	403	7/7	0.91	0.12	56,57,62,62	0
6	N2H	D	401	9/9	0.91	0.10	29,31,35,35	0
2	GOL	D	403	6/6	0.92	0.11	34,40,45,50	0
2	GOL	F	402	6/6	0.92	0.10	41,47,52,53	0
2	GOL	K	402	6/6	0.92	0.10	41,47,51,56	0
2	GOL	M	403	6/6	0.93	0.09	33,41,47,51	0
2	GOL	J	402	6/6	0.93	0.12	38,44,47,53	0
2	GOL	M	402	6/6	0.93	0.10	36,45,48,53	0
2	GOL	B	402	6/6	0.94	0.10	39,45,47,52	0
2	GOL	L	402	6/6	0.94	0.08	33,41,48,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	D	402	6/6	0.94	0.10	35,44,48,52	0
2	GOL	C	402	6/6	0.94	0.10	38,44,48,53	0
2	GOL	N	403	6/6	0.94	0.09	36,44,44,45	0
2	GOL	K	403	6/6	0.94	0.11	37,45,49,55	0
2	GOL	O	402	6/6	0.94	0.09	47,49,50,53	0
7	NA	L	404	1/1	0.94	0.10	52,52,52,52	0
2	GOL	N	402	6/6	0.95	0.09	39,49,52,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.