wwPDB X-ray Structure Validation Summary Report (i)

Apr 13, 2016 – 11:10 AM EDT

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

This is a 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

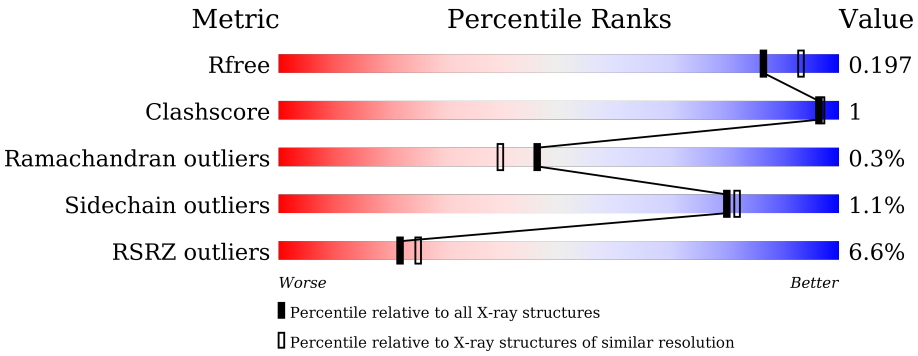
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027107
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027107

1 Overall quality at a glance (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}	91344	8664 (2.00-1.96)
Clashscore	102246	9905 (2.00-1.96)
Ramachandran outliers	100387	9792 (2.00-1.96)
Sidechain outliers	100360	9791 (2.00-1.96)
RSRZ outliers	91569	8679 (2.00-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	11% 92% 5%
1	B	304	4% 94%
1	C	304	3% 94% 5%
1	D	304	% 94%
1	E	304	% 96%
1	F	304	% 94%

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

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	402	-	-	-	X
2	GOL	B	403	-	-	-	X
2	GOL	C	403	-	-	-	X
2	GOL	C	405	-	-	-	X
2	GOL	D	403	-	-	-	X
2	GOL	E	403	-	-	-	X
2	GOL	E	404	-	-	-	X
2	GOL	E	405	-	-	-	X
2	GOL	F	402	-	-	-	X
2	GOL	F	403	-	-	-	X
2	GOL	I	401	-	-	-	X
2	GOL	J	402	-	-	-	X
2	GOL	J	403	-	-	-	X
2	GOL	J	404	-	-	-	X
2	GOL	J	405	-	-	-	X
2	GOL	K	402	-	-	-	X
2	GOL	K	403	-	-	-	X
2	GOL	K	404	-	-	-	X
2	GOL	L	402	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	M	403	-	-	-	X
2	GOL	N	403	-	-	-	X
2	GOL	N	404	-	-	-	X
3	PEG	A	404	-	-	-	X
3	PEG	D	404	-	-	-	X
3	PEG	D	405	-	-	-	X
3	PEG	L	403	-	-	-	X
4	PGE	C	406	-	-	-	X
4	PGE	J	407	-	-	-	X
5	EDO	A	406	-	-	-	X
5	EDO	C	407	-	-	-	X
5	EDO	D	406	-	-	-	X
5	EDO	K	405	-	-	-	X
5	EDO	N	405	-	-	-	X
5	EDO	P	401	-	-	-	X
6	N2H	F	401	-	-	-	X
6	N2H	G	401	-	-	-	X
6	N2H	M	401	-	-	-	X
6	N2H	N	401	-	-	-	X
6	N2H	O	401	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 42615 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called N-carbamoylputrescine amidohydrolase.

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

There are 48 discrepancies between the modelled and reference sequences:

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

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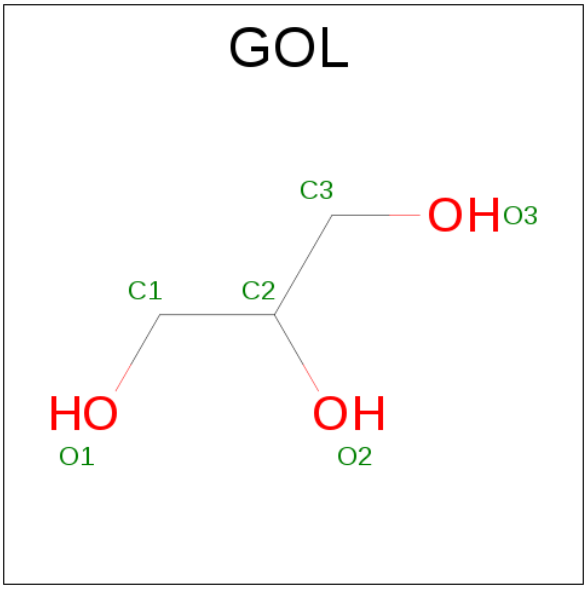
Chain	Residue	Modelled	Actual	Comment	Reference
O	-2	SER	-	expression tag	UNP G7ITU5
O	-1	ASN	-	expression tag	UNP G7ITU5
O	0	ALA	-	expression tag	UNP G7ITU5
P	-2	SER	-	expression tag	UNP G7ITU5
P	-1	ASN	-	expression tag	UNP G7ITU5
P	0	ALA	-	expression tag	UNP G7ITU5

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



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

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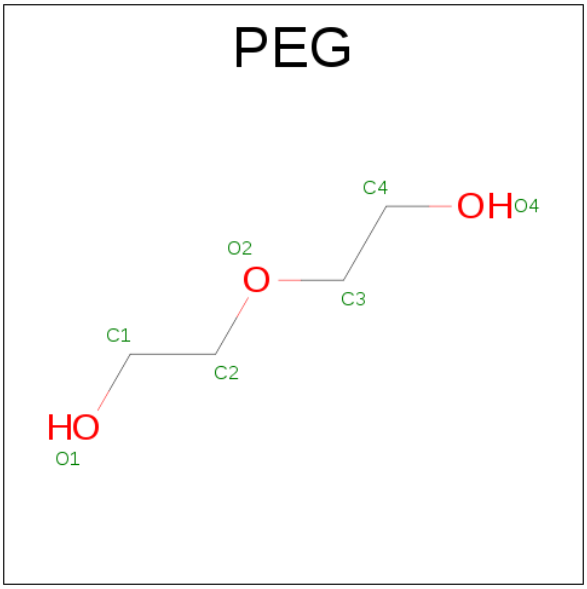
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	M	1	Total C O 6 3 3	0	0
2	M	1	Total C O 6 3 3	0	0
2	N	1	Total C O 6 3 3	0	0
2	N	1	Total C O 6 3 3	0	0
2	N	1	Total C O 6 3 3	0	0
2	O	1	Total C O 6 3 3	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

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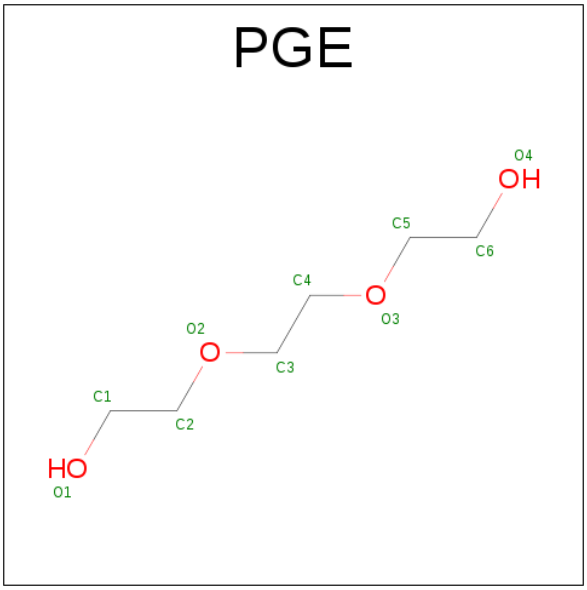
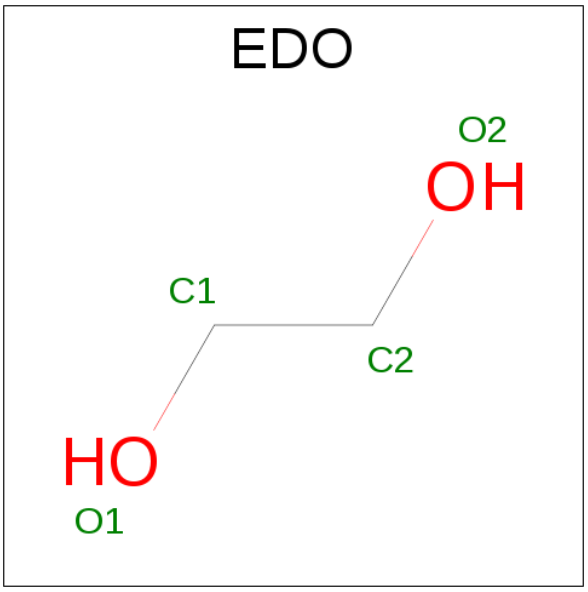
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	L	1	Total C O 7 4 3	0	0

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



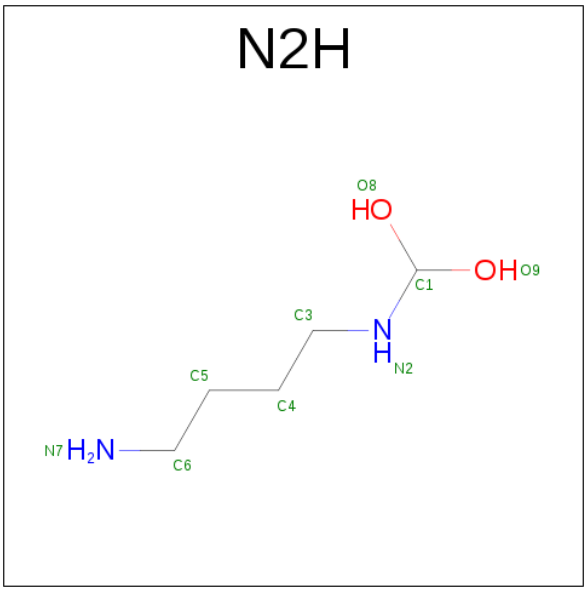
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 10 6 4	0	0
4	C	1	Total C O 10 6 4	0	0
4	G	1	Total C O 10 6 4	0	0
4	J	1	Total C O 10 6 4	0	0

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



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

- Molecule 6 is (4-azanylbutylamino)methanediol (three-letter code: N2H) (formula: $C_5H_{14}N_2O_2$).



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

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

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

- Molecule 8 is water.

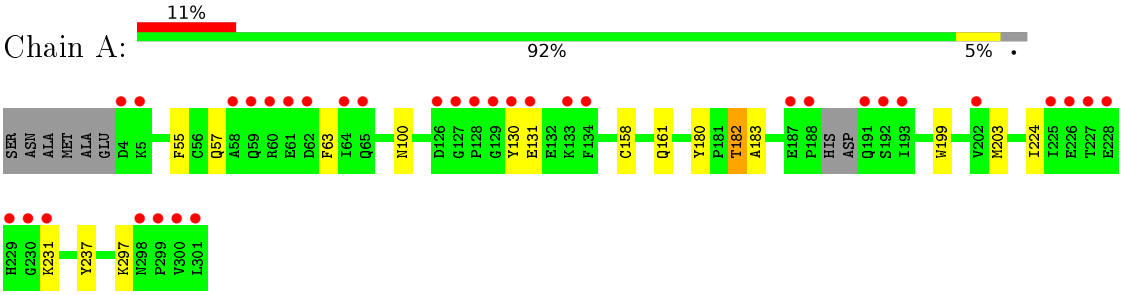
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	241	Total O 241 241	0	0
8	B	288	Total O 288 288	0	0
8	C	345	Total O 345 345	0	0
8	D	348	Total O 348 348	0	0
8	E	335	Total O 335 335	0	0
8	F	268	Total O 268 268	0	0
8	G	220	Total O 220 220	0	0
8	H	85	Total O 85 85	0	0
8	I	246	Total O 246 246	0	0
8	J	287	Total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

3 Residue-property plots (i)

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

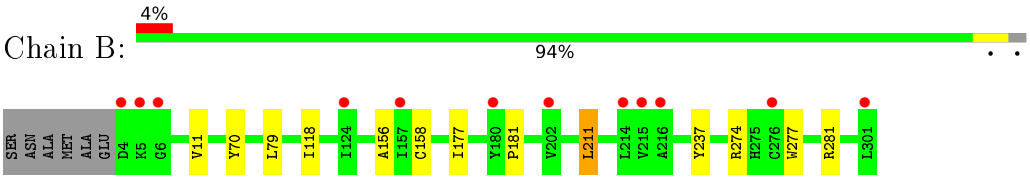
- Molecule 1: N-carbamoylputrescine amidohydrolase

Chain A:



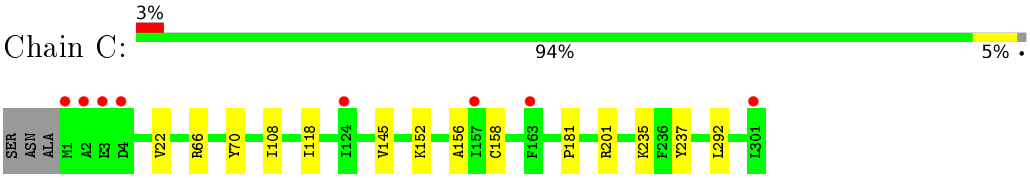
- Molecule 1: N-carbamoylputrescine amidohydrolase

Chain B:



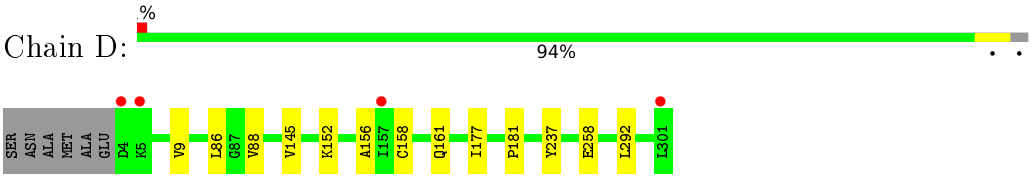
- Molecule 1: N-carbamoylputrescine amidohydrolase

Chain C:



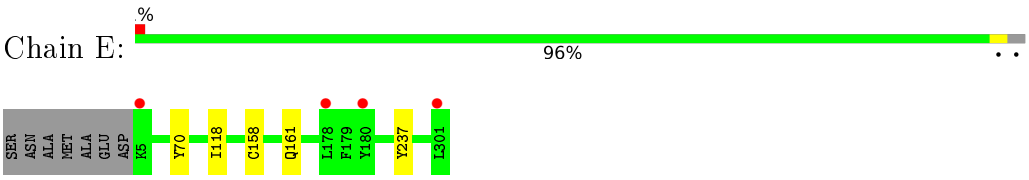
- Molecule 1: N-carbamoylputrescine amidohydrolase

Chain D:



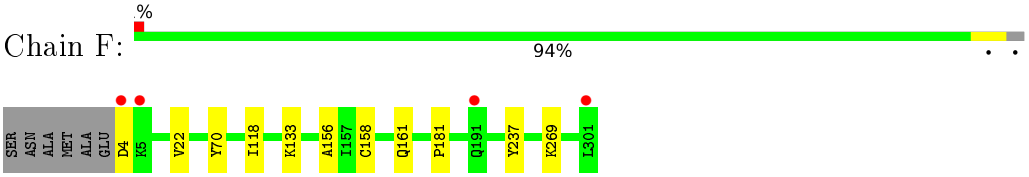
- Molecule 1: N-carbamoylputrescine amidohydrolase

Chain E:



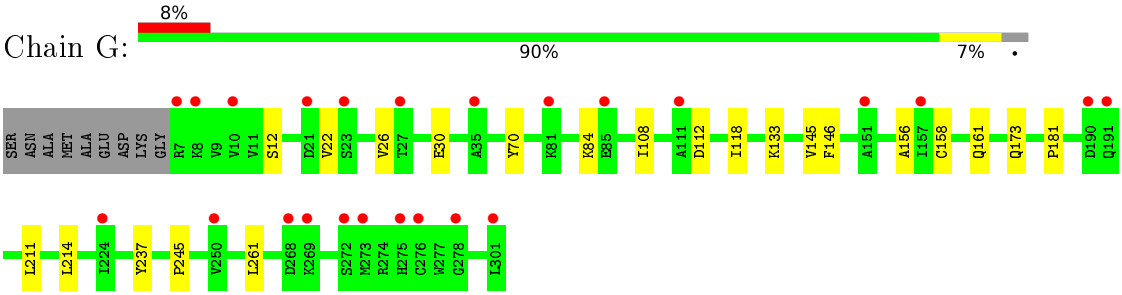
• Molecule 1: N-carbamoylputrescine amidohydrolase

Chain F:



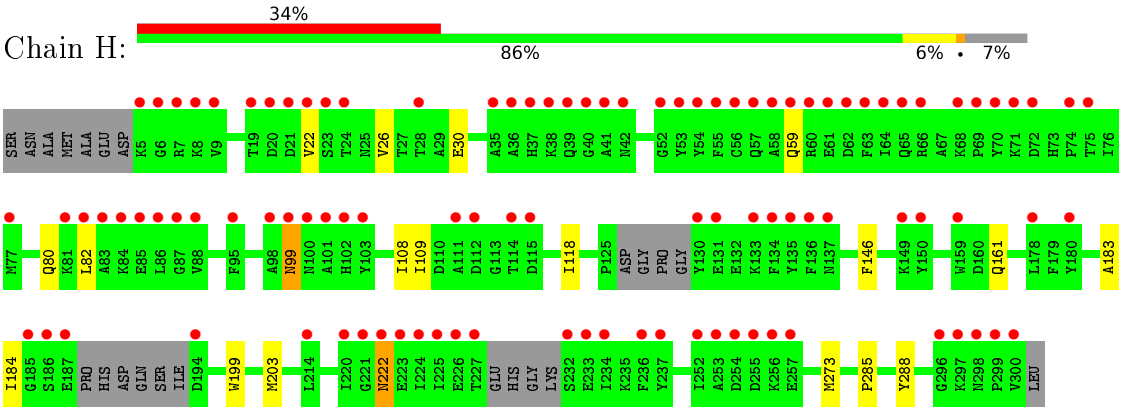
• Molecule 1: N-carbamoylputrescine amidohydrolase

Chain G:



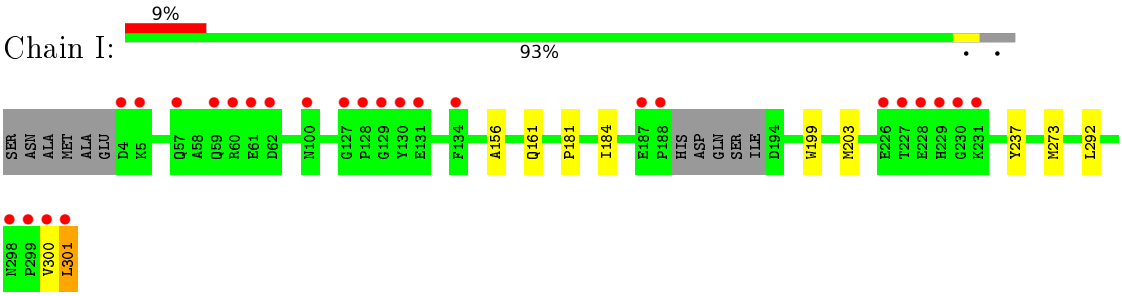
• Molecule 1: N-carbamoylputrescine amidohydrolase

Chain H:



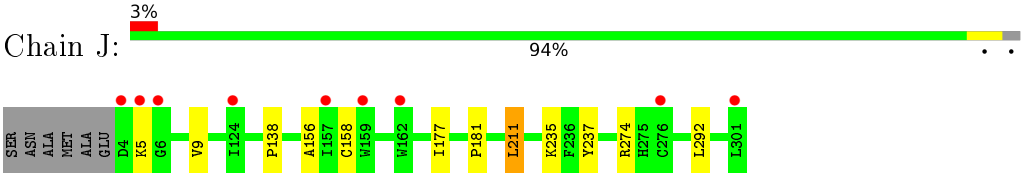
• Molecule 1: N-carbamoylputrescine amidohydrolase

Chain I:



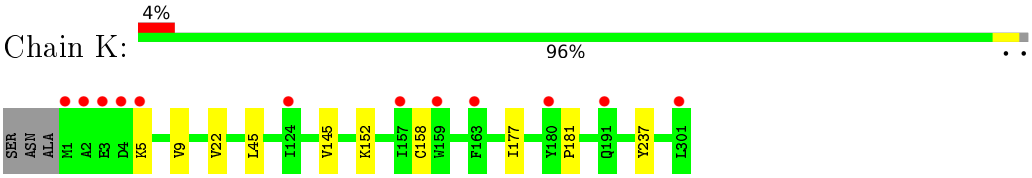
• Molecule 1: N-carbamoylputrescine amidohydrolase

Chain J:



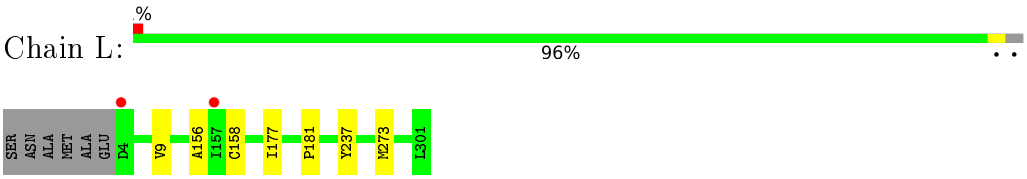
• Molecule 1: N-carbamoylputrescine amidohydrolase

Chain K:



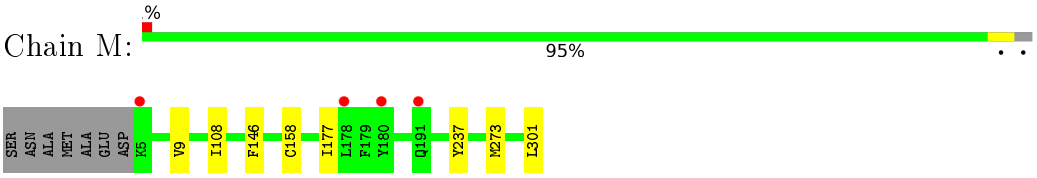
• Molecule 1: N-carbamoylputrescine amidohydrolase

Chain L:



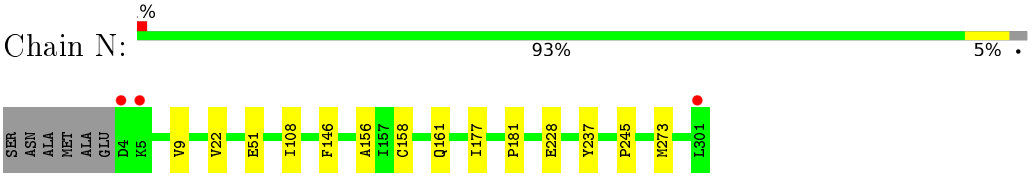
• Molecule 1: N-carbamoylputrescine amidohydrolase

Chain M:



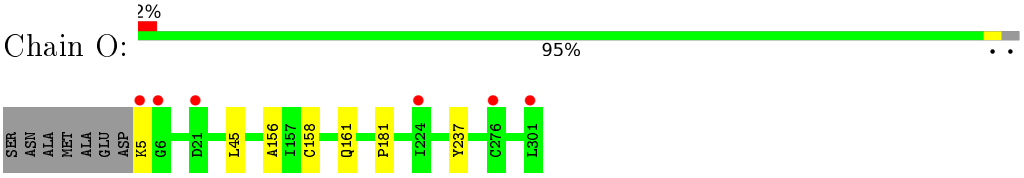
• Molecule 1: N-carbamoylputrescine amidohydrolase

Chain N:



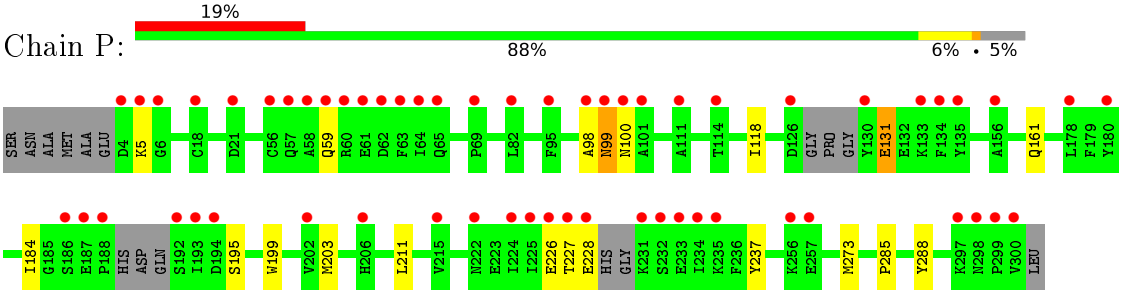
• Molecule 1: N-carbamoylputrescine amidohydrolase

Chain O:



• Molecule 1: N-carbamoylputrescine amidohydrolase

Chain P:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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%)	DCC
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 , 51.5	EDS
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	6 of 462097 reflections (0.001%)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

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

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

The worst 5 of 104 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:228:GLU:HB3	8:N:688:HOH:O	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:145[B]:VAL:CG1	1:D:152:LYS:HG2	2.28	0.63
1:D:258:GLU:H	3:D:405:PEG:H21	1.63	0.63
1:P:99:ASN:HD22	1:P:100:ASN:H	1.47	0.63
1:D:86:LEU:HB2	1:D:88[B]:VAL:HG12	1.82	0.61

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	295/304 (97%)	282 (96%)	13 (4%)	0	100	100
1	B	298/304 (98%)	287 (96%)	10 (3%)	1 (0%)	46	39
1	C	303/304 (100%)	294 (97%)	8 (3%)	1 (0%)	46	39
1	D	301/304 (99%)	294 (98%)	6 (2%)	1 (0%)	46	39
1	E	298/304 (98%)	287 (96%)	10 (3%)	1 (0%)	46	39
1	F	300/304 (99%)	287 (96%)	12 (4%)	1 (0%)	46	39
1	G	294/304 (97%)	283 (96%)	10 (3%)	1 (0%)	46	39
1	H	276/304 (91%)	265 (96%)	9 (3%)	2 (1%)	26	17
1	I	290/304 (95%)	280 (97%)	10 (3%)	0	100	100
1	J	300/304 (99%)	292 (97%)	7 (2%)	1 (0%)	46	39
1	K	304/304 (100%)	293 (96%)	10 (3%)	1 (0%)	46	39
1	L	300/304 (99%)	289 (96%)	10 (3%)	1 (0%)	46	39
1	M	300/304 (99%)	292 (97%)	7 (2%)	1 (0%)	46	39
1	N	300/304 (99%)	289 (96%)	10 (3%)	1 (0%)	46	39
1	O	297/304 (98%)	288 (97%)	8 (3%)	1 (0%)	46	39
1	P	283/304 (93%)	277 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	4739/4864 (97%)	4579 (97%)	146 (3%)	14 (0%)	46 39

5 of 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

5.3.2 Protein sidechains (i)

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%)	63 63
1	B	250/252 (99%)	247 (99%)	3 (1%)	78 80
1	C	254/252 (101%)	252 (99%)	2 (1%)	86 88
1	D	253/252 (100%)	251 (99%)	2 (1%)	86 88
1	E	250/252 (99%)	248 (99%)	2 (1%)	86 88
1	F	252/252 (100%)	250 (99%)	2 (1%)	86 88
1	G	247/252 (98%)	245 (99%)	2 (1%)	86 88
1	H	237/252 (94%)	234 (99%)	3 (1%)	76 77
1	I	244/252 (97%)	240 (98%)	4 (2%)	70 71
1	J	252/252 (100%)	249 (99%)	3 (1%)	78 80
1	K	255/252 (101%)	253 (99%)	2 (1%)	86 88
1	L	252/252 (100%)	251 (100%)	1 (0%)	93 95
1	M	252/252 (100%)	250 (99%)	2 (1%)	86 88
1	N	252/252 (100%)	250 (99%)	2 (1%)	86 88
1	O	249/252 (99%)	246 (99%)	3 (1%)	78 80
1	P	243/252 (96%)	238 (98%)	5 (2%)	61 61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3991/4032 (99%)	3948 (99%)	43 (1%)	80 82

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	118	ILE
1	I	301	LEU
1	P	118	ILE
1	H	222	ASN
1	I	184	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	65	GLN
1	J	173	GLN
1	O	65	GLN
1	H	99	ASN
1	I	161	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 64 ligands modelled in this entry, 1 is monoatomic - leaving 63 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link

column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GOL	A	401	-	5,5,5	0.33	0	5,5,5	0.26	0
2	GOL	A	402	-	5,5,5	0.37	0	5,5,5	0.41	0
2	GOL	A	403	-	5,5,5	0.29	0	5,5,5	0.32	0
3	PEG	A	404	-	6,6,6	0.53	0	5,5,5	0.22	0
4	PGE	A	405	-	9,9,9	0.56	0	8,8,8	0.48	0
5	EDO	A	406	-	3,3,3	0.51	0	2,2,2	0.34	0
6	N2H	B	401	1	5,8,8	1.55	1 (20%)	4,8,8	1.31	1 (25%)
2	GOL	B	402	-	5,5,5	0.12	0	5,5,5	0.53	0
2	GOL	B	403	-	5,5,5	0.36	0	5,5,5	0.42	0
6	N2H	C	401	1	5,8,8	2.17	1 (20%)	4,8,8	1.61	1 (25%)
2	GOL	C	402	-	5,5,5	0.61	0	5,5,5	0.47	0
2	GOL	C	403	-	5,5,5	0.22	0	5,5,5	0.33	0
2	GOL	C	404	-	5,5,5	0.30	0	5,5,5	0.36	0
2	GOL	C	405	-	5,5,5	0.29	0	5,5,5	0.41	0
4	PGE	C	406	-	9,9,9	0.56	0	8,8,8	0.26	0
5	EDO	C	407	-	3,3,3	0.59	0	2,2,2	0.09	0
6	N2H	D	401	1	5,8,8	1.81	1 (20%)	4,8,8	1.64	1 (25%)
2	GOL	D	402	-	5,5,5	0.44	0	5,5,5	1.00	0
2	GOL	D	403	-	5,5,5	0.35	0	5,5,5	0.39	0
3	PEG	D	404	-	6,6,6	0.50	0	5,5,5	0.39	0
3	PEG	D	405	-	6,6,6	0.49	0	5,5,5	0.66	0
5	EDO	D	406	-	3,3,3	0.52	0	2,2,2	0.17	0
6	N2H	E	401	1	5,8,8	1.84	1 (20%)	4,8,8	1.34	1 (25%)
2	GOL	E	402	-	5,5,5	0.43	0	5,5,5	0.37	0
2	GOL	E	403	-	5,5,5	0.44	0	5,5,5	0.24	0
2	GOL	E	404	-	5,5,5	0.27	0	5,5,5	0.33	0
2	GOL	E	405	-	5,5,5	0.43	0	5,5,5	0.25	0
6	N2H	F	401	1	5,8,8	2.31	1 (20%)	4,8,8	1.19	1 (25%)
2	GOL	F	402	-	5,5,5	0.30	0	5,5,5	0.12	0
2	GOL	F	403	-	5,5,5	0.56	0	5,5,5	0.79	0
6	N2H	G	401	1	5,8,8	2.88	1 (20%)	4,8,8	1.33	1 (25%)
2	GOL	G	402	-	5,5,5	0.33	0	5,5,5	0.24	0
3	PEG	G	403	-	6,6,6	0.52	0	5,5,5	0.25	0
4	PGE	G	404	-	9,9,9	0.50	0	8,8,8	0.28	0
2	GOL	H	401	-	5,5,5	0.35	0	5,5,5	0.69	0
2	GOL	I	401	-	5,5,5	0.38	0	5,5,5	0.26	0
2	GOL	I	402	-	5,5,5	0.62	0	5,5,5	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	N2H	J	401	1	5,8,8	2.82	1 (20%)	4,8,8	1.29	1 (25%)
2	GOL	J	402	-	5,5,5	0.29	0	5,5,5	0.31	0
2	GOL	J	403	-	5,5,5	0.45	0	5,5,5	0.35	0
2	GOL	J	404	-	5,5,5	0.18	0	5,5,5	0.42	0
2	GOL	J	405	-	5,5,5	0.65	0	5,5,5	1.13	1 (20%)
3	PEG	J	406	-	6,6,6	0.54	0	5,5,5	0.30	0
4	PGE	J	407	-	9,9,9	0.59	0	8,8,8	0.35	0
6	N2H	K	401	1	5,8,8	2.25	1 (20%)	4,8,8	1.67	1 (25%)
2	GOL	K	402	-	5,5,5	0.22	0	5,5,5	0.55	0
2	GOL	K	403	-	5,5,5	0.46	0	5,5,5	0.46	0
2	GOL	K	404	-	5,5,5	0.17	0	5,5,5	0.15	0
5	EDO	K	405	-	3,3,3	0.55	0	2,2,2	0.15	0
6	N2H	L	401	1	5,8,8	1.49	1 (20%)	4,8,8	1.46	1 (25%)
2	GOL	L	402	-	5,5,5	0.24	0	5,5,5	0.22	0
3	PEG	L	403	-	6,6,6	0.52	0	5,5,5	0.37	0
6	N2H	M	401	1	5,8,8	1.55	1 (20%)	4,8,8	1.20	1 (25%)
2	GOL	M	402	-	5,5,5	0.28	0	5,5,5	0.46	0
2	GOL	M	403	-	5,5,5	0.35	0	5,5,5	0.08	0
6	N2H	N	401	1	5,8,8	1.97	1 (20%)	4,8,8	1.35	1 (25%)
2	GOL	N	402	-	5,5,5	0.41	0	5,5,5	0.61	0
2	GOL	N	403	-	5,5,5	0.31	0	5,5,5	0.15	0
2	GOL	N	404	-	5,5,5	0.36	0	5,5,5	0.43	0
5	EDO	N	405	-	3,3,3	0.46	0	2,2,2	0.32	0
6	N2H	O	401	1	5,8,8	1.88	1 (20%)	4,8,8	1.05	0
2	GOL	O	402	-	5,5,5	0.05	0	5,5,5	0.50	0
5	EDO	P	401	-	3,3,3	0.56	0	2,2,2	0.21	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
2	GOL	A	402	-	-	0/4/4/4	0/0/0/0
2	GOL	A	403	-	-	0/4/4/4	0/0/0/0
3	PEG	A	404	-	-	0/4/4/4	0/0/0/0
4	PGE	A	405	-	-	0/7/7/7	0/0/0/0
5	EDO	A	406	-	-	0/1/1/1	0/0/0/0
6	N2H	B	401	1	-	0/4/6/6	0/0/0/0
2	GOL	B	402	-	-	0/4/4/4	0/0/0/0

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	L	402	-	-	0/4/4/4	0/0/0/0
3	PEG	L	403	-	-	0/4/4/4	0/0/0/0
6	N2H	M	401	1	-	0/4/6/6	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
6	N2H	N	401	1	-	0/4/6/6	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
5	EDO	N	405	-	-	0/1/1/1	0/0/0/0
6	N2H	O	401	1	-	0/4/6/6	0/0/0/0
2	GOL	O	402	-	-	0/4/4/4	0/0/0/0
5	EDO	P	401	-	-	0/1/1/1	0/0/0/0

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	401	N2H	C3-N2	2.85	1.50	1.46
6	M	401	N2H	C3-N2	3.16	1.50	1.46
6	B	401	N2H	C3-N2	3.19	1.50	1.46
6	D	401	N2H	C3-N2	3.81	1.51	1.46
6	E	401	N2H	C3-N2	3.85	1.51	1.46

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	401	N2H	C4-C3-N2	-3.11	104.49	112.04
6	K	401	N2H	C4-C3-N2	-3.08	104.56	112.04
6	C	401	N2H	C4-C3-N2	-2.89	105.03	112.04
6	L	401	N2H	C4-C3-N2	-2.63	105.66	112.04
6	E	401	N2H	C4-C3-N2	-2.41	106.20	112.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	404	GOL	1	0
2	C	405	GOL	1	0
3	D	405	PEG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	401	GOL	2	0
2	J	405	GOL	1	0
2	O	402	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, 95^{th} 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%)	0.33	34 (11%) 6 8	19, 32, 76, 95	0
1	B	298/304 (98%)	0.05	12 (4%) 42 46	17, 26, 43, 85	0
1	C	301/304 (99%)	-0.04	8 (2%) 58 61	16, 25, 38, 82	0
1	D	298/304 (98%)	-0.16	4 (1%) 79 82	16, 24, 36, 71	0
1	E	297/304 (97%)	-0.12	4 (1%) 79 82	17, 26, 38, 66	0
1	F	298/304 (98%)	-0.27	4 (1%) 79 82	17, 30, 43, 79	0
1	G	295/304 (97%)	0.54	24 (8%) 15 17	29, 42, 58, 70	0
1	H	282/304 (92%)	1.70	103 (36%) 0 1	32, 57, 91, 106	0
1	I	293/304 (96%)	0.21	26 (8%) 12 14	20, 30, 69, 113	0
1	J	298/304 (98%)	0.01	9 (3%) 54 57	17, 26, 41, 96	0
1	K	301/304 (99%)	0.00	12 (3%) 42 46	16, 28, 41, 86	0
1	L	298/304 (98%)	-0.18	2 (0%) 89 90	16, 24, 36, 76	0
1	M	297/304 (97%)	-0.12	4 (1%) 79 82	16, 24, 36, 59	0
1	N	298/304 (98%)	-0.29	3 (1%) 84 86	16, 25, 37, 69	0
1	O	297/304 (97%)	-0.05	6 (2%) 68 71	22, 35, 50, 78	0
1	P	289/304 (95%)	1.01	58 (20%) 1 1	23, 47, 87, 100	0
All	All	4736/4864 (97%)	0.16	313 (6%) 22 25	16, 29, 63, 113	0

The worst 5 of 313 RSRZ outliers are listed below:

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

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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
3	PEG	D	405	7/7	0.73	0.39	11.02	63,63,70,71	0
2	GOL	E	404	6/6	0.95	0.21	10.02	34,41,42,45	0
2	GOL	I	401	6/6	0.91	0.18	9.41	44,45,48,50	0
2	GOL	N	404	6/6	0.85	0.34	9.30	55,56,59,60	0
2	GOL	M	403	6/6	0.96	0.20	9.11	33,41,47,51	0
2	GOL	F	402	6/6	0.93	0.26	8.94	41,47,52,53	0
2	GOL	J	403	6/6	0.85	0.21	8.69	43,49,51,52	0
2	GOL	K	404	6/6	0.96	0.24	8.59	41,46,50,54	0
2	GOL	C	403	6/6	0.94	0.22	8.46	35,44,48,53	0
2	GOL	L	402	6/6	0.97	0.18	7.05	33,41,48,56	0
3	PEG	D	404	7/7	0.88	0.29	6.86	58,60,61,61	0
2	GOL	N	403	6/6	0.94	0.21	5.97	36,44,44,45	0
2	GOL	A	401	6/6	0.87	0.18	5.42	50,54,59,60	0
2	GOL	C	405	6/6	0.85	0.36	5.38	37,50,54,54	0
4	PGE	C	406	10/10	0.88	0.26	5.16	59,61,64,68	0
3	PEG	L	403	7/7	0.88	0.33	5.09	56,57,62,62	0
2	GOL	J	402	6/6	0.90	0.17	4.55	38,44,47,53	0
5	EDO	D	406	4/4	0.89	0.25	4.13	53,54,55,55	0
2	GOL	E	405	6/6	0.75	0.33	3.88	59,64,66,66	0
5	EDO	N	405	4/4	0.83	0.23	3.86	52,53,54,54	0
5	EDO	C	407	4/4	0.86	0.22	3.74	44,47,48,50	0
5	EDO	K	405	4/4	0.84	0.20	3.59	44,50,51,56	0
2	GOL	E	403	6/6	0.89	0.18	3.56	49,58,64,71	0
5	EDO	A	406	4/4	0.90	0.22	3.44	50,50,51,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	N2H	N	401	9/9	0.88	0.20	3.43	33,35,38,42	0
2	GOL	B	402	6/6	0.92	0.14	3.42	39,45,47,52	0
6	N2H	O	401	9/9	0.88	0.18	3.39	41,43,45,51	0
2	GOL	K	403	6/6	0.93	0.14	3.39	37,45,49,55	0
2	GOL	B	403	6/6	0.83	0.18	3.32	46,56,58,59	0
3	PEG	A	404	7/7	0.84	0.27	3.23	68,69,71,71	0
2	GOL	J	404	6/6	0.84	0.20	3.09	53,59,61,61	0
2	GOL	J	405	6/6	0.91	0.23	3.04	29,33,38,39	6
4	PGE	J	407	10/10	0.79	0.30	2.85	50,68,73,75	0
6	N2H	M	401	9/9	0.90	0.20	2.72	24,27,35,37	0
5	EDO	P	401	4/4	0.90	0.17	2.66	49,51,52,54	0
2	GOL	D	403	6/6	0.91	0.20	2.60	34,40,45,50	0
2	GOL	K	402	6/6	0.92	0.18	2.44	41,47,51,56	0
2	GOL	F	403	6/6	0.88	0.17	2.24	36,46,48,48	0
6	N2H	G	401	9/9	0.91	0.16	2.10	44,45,45,46	0
6	N2H	F	401	9/9	0.90	0.16	2.06	39,40,41,45	0
2	GOL	C	404	6/6	0.89	0.17	1.98	48,56,59,60	0
2	GOL	I	402	6/6	0.84	0.19	1.84	36,44,45,46	0
2	GOL	D	402	6/6	0.95	0.13	1.72	35,44,48,52	0
6	N2H	E	401	9/9	0.92	0.18	1.68	31,32,36,38	0
2	GOL	E	402	6/6	0.92	0.13	1.57	40,50,54,58	0
6	N2H	J	401	9/9	0.93	0.20	1.56	29,33,35,36	0
6	N2H	B	401	9/9	0.91	0.20	1.52	30,33,37,37	0
6	N2H	D	401	9/9	0.94	0.18	1.52	29,31,35,35	0
6	N2H	L	401	9/9	0.93	0.18	1.45	28,32,36,38	0
2	GOL	C	402	6/6	0.94	0.13	1.33	38,44,48,53	0
6	N2H	K	401	9/9	0.91	0.20	1.26	31,32,39,41	0
6	N2H	C	401	9/9	0.93	0.19	1.22	28,30,36,38	0
4	PGE	A	405	10/10	0.77	0.19	1.14	46,61,66,68	0
2	GOL	N	402	6/6	0.92	0.13	0.83	39,49,52,56	0
2	GOL	O	402	6/6	0.93	0.12	0.81	47,49,50,53	0
2	GOL	G	402	6/6	0.93	0.12	0.78	43,47,50,50	0
2	GOL	H	401	6/6	0.92	0.14	0.59	57,61,62,63	0
2	GOL	M	402	6/6	0.96	0.09	-0.17	36,45,48,53	0
2	GOL	A	403	6/6	0.86	0.15	-0.19	59,64,67,68	0
7	NA	L	404	1/1	0.88	0.24	-	52,52,52,52	0
2	GOL	A	402	6/6	0.78	0.29	-	56,59,61,61	0
4	PGE	G	404	10/10	0.76	0.28	-	64,88,100,103	0
3	PEG	J	406	7/7	0.78	0.27	-	68,70,72,72	0
3	PEG	G	403	7/7	0.72	0.25	-	66,70,73,74	0

6.5 Other polymers (i)

There are no such residues in this entry.