Full wwPDB X-ray Structure Validation Report (i)

Apr 13, 2016 – 11:23 AM EDT

PDB ID	:	5H8L
Title	:	Crystal structure of Medicago truncatula N-carbamoylputrescine amidohydrolase (MtCPA) C158S mutant in complex with putrescine
Authors	:	Sekula, B.; Ruszkowski, M.; Malinska, M.; Dauter, Z.
Deposited on	:	2015-12-23
Resolution	:	2.29 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
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:

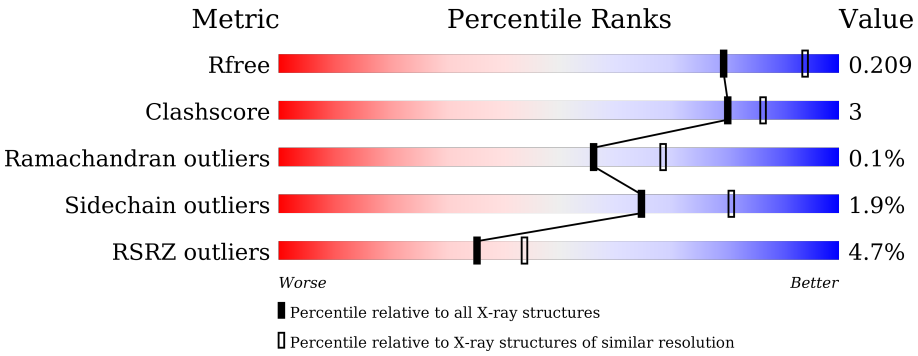
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027107
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.29 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	7% 81% 13%
1	B	304	2% 90% 8%
1	C	304	% 92% 6%
1	D	304	91% 7%
1	E	304	% 93%
1	F	304	% 89% 8%

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Mol	Chain	Length	Quality of chain
1	G	304	6% 84% 13%
1	H	304	28% 79% 13% 7%
1	I	304	5% 89% 6%
1	J	304	2% 91% 7%
1	K	304	3% 92% 7%
1	L	304	93% 5%
1	M	304	89% 9%
1	N	304	92% 6%
1	O	304	2% 90% 7%
1	P	304	13% 88% 5% 6%

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	A	402	-	-	-	X
2	GOL	C	403	-	-	-	X
2	GOL	D	403	-	-	-	X
2	GOL	E	404	-	-	-	X
2	GOL	E	405	-	-	-	X
2	GOL	F	402	-	-	-	X
2	GOL	I	401	-	-	-	X
2	GOL	J	403	-	-	-	X
2	GOL	J	404	-	-	-	X
2	GOL	K	404	-	-	-	X
2	GOL	L	402	-	-	X	X
2	GOL	M	402	-	-	-	X
2	GOL	N	404	-	-	-	X
2	GOL	N	405	-	-	-	X
2	GOL	P	401	-	-	-	X
3	EDO	C	404	-	-	-	X
3	EDO	D	404	-	-	-	X
3	EDO	F	403	-	-	-	X
3	EDO	K	405	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	L	403	-	-	-	X
3	EDO	M	403	-	-	-	X
3	EDO	N	406	-	-	-	X
3	EDO	P	403	-	-	-	X
4	PUT	B	401	-	-	-	X
4	PUT	C	401	-	-	-	X
4	PUT	D	402	-	-	-	X
4	PUT	E	401	-	-	-	X
4	PUT	F	401	-	-	-	X
4	PUT	G	401	-	-	-	X
4	PUT	J	401	-	-	-	X
4	PUT	K	401	-	-	-	X
4	PUT	L	401	-	-	-	X
4	PUT	M	401	-	-	-	X
4	PUT	N	402	-	-	-	X
4	PUT	O	401	-	-	-	X
5	PEG	D	406	-	-	-	X
5	PEG	K	406	-	-	-	X
5	PEG	L	405	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 41665 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	295	Total	C	N	O	S	0	2	0
			2347	1501	404	433	9			
1	B	298	Total	C	N	O	S	0	1	0
			2372	1514	411	440	7			
1	C	301	Total	C	N	O	S	0	1	0
			2390	1524	412	445	9			
1	D	298	Total	C	N	O	S	0	2	0
			2372	1515	409	440	8			
1	E	297	Total	C	N	O	S	0	0	0
			2357	1505	408	437	7			
1	F	298	Total	C	N	O	S	0	1	0
			2368	1511	409	440	8			
1	G	295	Total	C	N	O	S	0	0	0
			2344	1497	405	435	7			
1	H	282	Total	C	N	O	S	0	1	0
			2248	1440	387	413	8			
1	I	292	Total	C	N	O	S	0	1	0
			2318	1481	400	429	8			
1	J	298	Total	C	N	O	S	0	1	0
			2368	1511	409	440	8			
1	K	301	Total	C	N	O	S	0	1	0
			2390	1524	412	445	9			
1	L	298	Total	C	N	O	S	0	2	0
			2372	1515	409	440	8			
1	M	297	Total	C	N	O	S	0	2	0
			2364	1511	408	437	8			
1	N	298	Total	C	N	O	S	0	0	0
			2365	1509	409	440	7			
1	O	297	Total	C	N	O	S	0	1	0
			2360	1507	408	437	8			
1	P	287	Total	C	N	O	S	0	1	0
			2284	1463	393	420	8			

There are 64 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
A	158	SER	CYS	engineered mutation	UNP G7ITU5
B	-2	SER	-	expression tag	UNP G7ITU5
B	-1	ASN	-	expression tag	UNP G7ITU5
B	0	ALA	-	expression tag	UNP G7ITU5
B	158	SER	CYS	engineered mutation	UNP G7ITU5
C	-2	SER	-	expression tag	UNP G7ITU5
C	-1	ASN	-	expression tag	UNP G7ITU5
C	0	ALA	-	expression tag	UNP G7ITU5
C	158	SER	CYS	engineered mutation	UNP G7ITU5
D	-2	SER	-	expression tag	UNP G7ITU5
D	-1	ASN	-	expression tag	UNP G7ITU5
D	0	ALA	-	expression tag	UNP G7ITU5
D	158	SER	CYS	engineered mutation	UNP G7ITU5
E	-2	SER	-	expression tag	UNP G7ITU5
E	-1	ASN	-	expression tag	UNP G7ITU5
E	0	ALA	-	expression tag	UNP G7ITU5
E	158	SER	CYS	engineered mutation	UNP G7ITU5
F	-2	SER	-	expression tag	UNP G7ITU5
F	-1	ASN	-	expression tag	UNP G7ITU5
F	0	ALA	-	expression tag	UNP G7ITU5
F	158	SER	CYS	engineered mutation	UNP G7ITU5
G	-2	SER	-	expression tag	UNP G7ITU5
G	-1	ASN	-	expression tag	UNP G7ITU5
G	0	ALA	-	expression tag	UNP G7ITU5
G	158	SER	CYS	engineered mutation	UNP G7ITU5
H	-2	SER	-	expression tag	UNP G7ITU5
H	-1	ASN	-	expression tag	UNP G7ITU5
H	0	ALA	-	expression tag	UNP G7ITU5
H	158	SER	CYS	engineered mutation	UNP G7ITU5
I	-2	SER	-	expression tag	UNP G7ITU5
I	-1	ASN	-	expression tag	UNP G7ITU5
I	0	ALA	-	expression tag	UNP G7ITU5
I	158	SER	CYS	engineered mutation	UNP G7ITU5
J	-2	SER	-	expression tag	UNP G7ITU5
J	-1	ASN	-	expression tag	UNP G7ITU5
J	0	ALA	-	expression tag	UNP G7ITU5
J	158	SER	CYS	engineered mutation	UNP G7ITU5
K	-2	SER	-	expression tag	UNP G7ITU5
K	-1	ASN	-	expression tag	UNP G7ITU5

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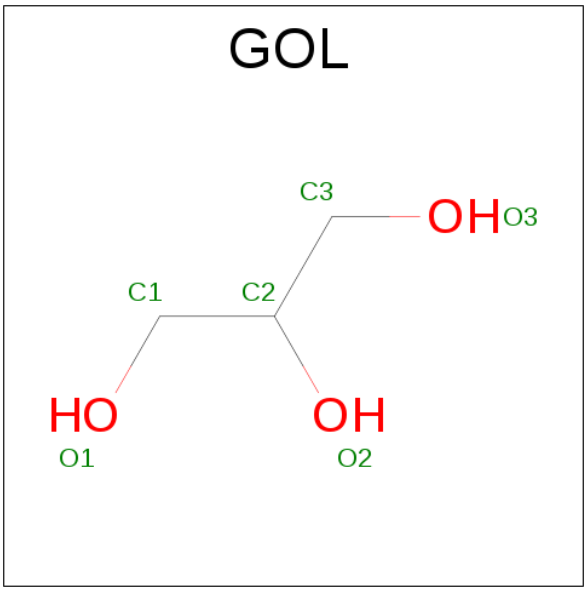
Chain	Residue	Modelled	Actual	Comment	Reference
K	0	ALA	-	expression tag	UNP G7ITU5
K	158	SER	CYS	engineered mutation	UNP G7ITU5
L	-2	SER	-	expression tag	UNP G7ITU5
L	-1	ASN	-	expression tag	UNP G7ITU5
L	0	ALA	-	expression tag	UNP G7ITU5
L	158	SER	CYS	engineered mutation	UNP G7ITU5
M	-2	SER	-	expression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

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



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

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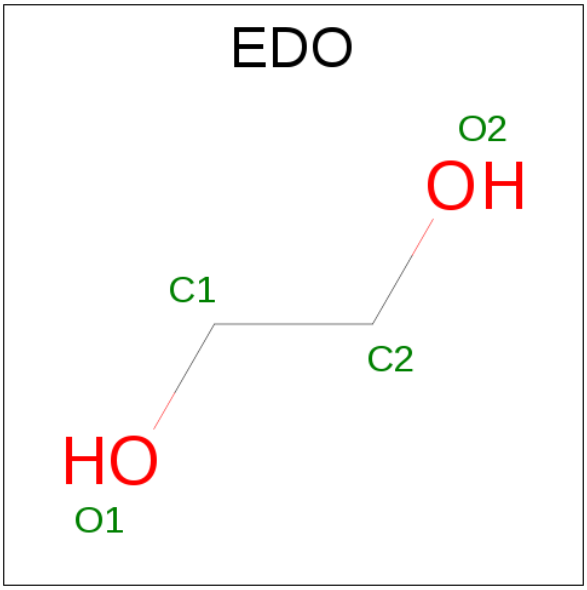
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	L	1	Total C O 6 3 3	0	0
2	M	1	Total C O 6 3 3	0	0
2	N	1	Total C O 6 3 3	0	0
2	N	1	Total C O 6 3 3	0	0
2	N	1	Total C O 6 3 3	0	0
2	N	1	Total C O 6 3 3	0	0
2	O	1	Total C O 6 3 3	0	0
2	P	1	Total C O 6 3 3	0	0

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



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

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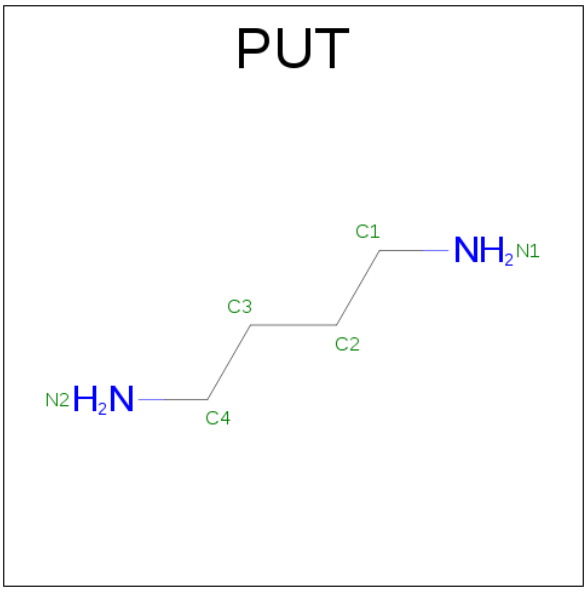
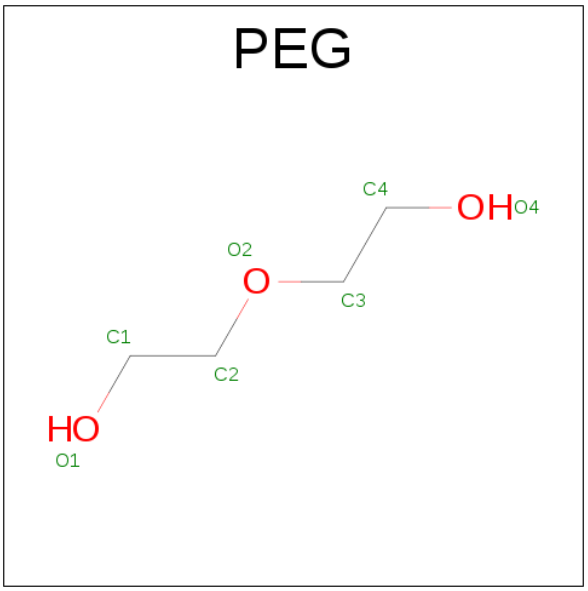
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		
3	I	1	Total	C	O	0	0
			4	2	2		
3	I	1	Total	C	O	0	0
			4	2	2		
3	K	1	Total	C	O	0	0
			4	2	2		
3	L	1	Total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

- Molecule 4 is 1,4-DIAMINOBUTANE (three-letter code: PUT) (formula: $C_4H_{12}N_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N 6 4 2	0	0
4	C	1	Total C N 6 4 2	0	0
4	D	1	Total C N 6 4 2	0	0
4	E	1	Total C N 6 4 2	0	0
4	F	1	Total C N 6 4 2	0	0
4	G	1	Total C N 6 4 2	0	0
4	J	1	Total C N 6 4 2	0	0
4	K	1	Total C N 6 4 2	0	0
4	L	1	Total C N 6 4 2	0	0
4	M	1	Total C N 6 4 2	0	0
4	N	1	Total C N 6 4 2	0	0
4	O	1	Total C N 6 4 2	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	194	Total O 194 194	0	0
6	B	264	Total O 264 264	0	0
6	C	291	Total O 291 291	0	0
6	D	312	Total O 312 312	0	0
6	E	274	Total O 274 274	0	0
6	F	205	Total O 205 205	0	0
6	G	169	Total O 169 169	0	0
6	H	61	Total O 61 61	0	0
6	I	214	Total O 214 214	0	0

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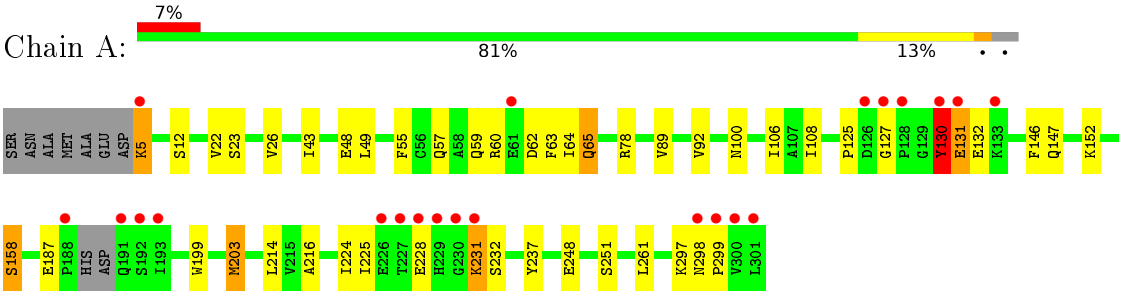
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	J	257	Total O 257 257	0	0
6	K	270	Total O 270 270	0	0
6	L	292	Total O 292 292	0	0
6	M	279	Total O 279 279	0	0
6	N	291	Total O 291 291	0	0
6	O	226	Total O 226 226	0	0
6	P	106	Total O 106 106	0	0

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.

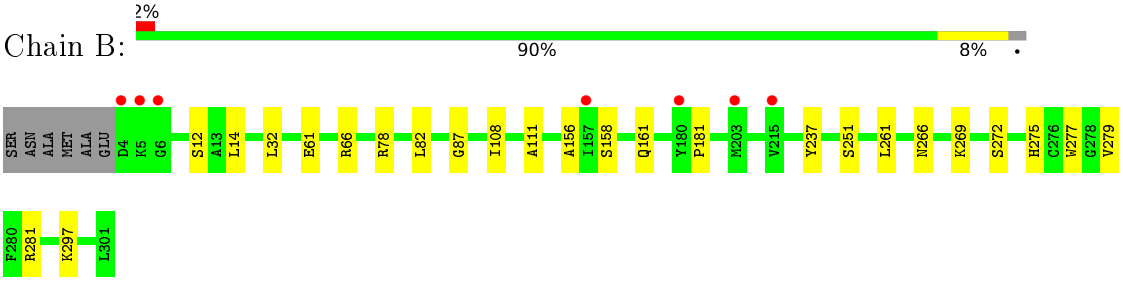
- Molecule 1: N-carbamoylputrescine amidohydrolase

Chain A:



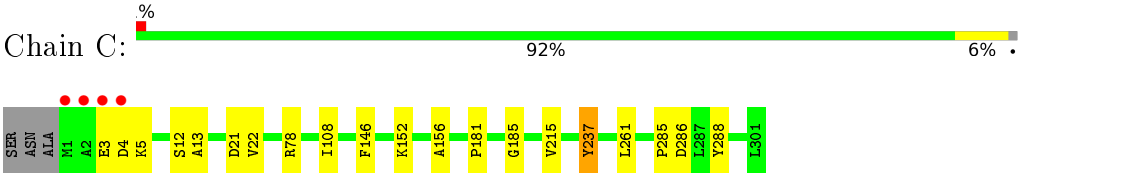
- Molecule 1: N-carbamoylputrescine amidohydrolase

Chain B:



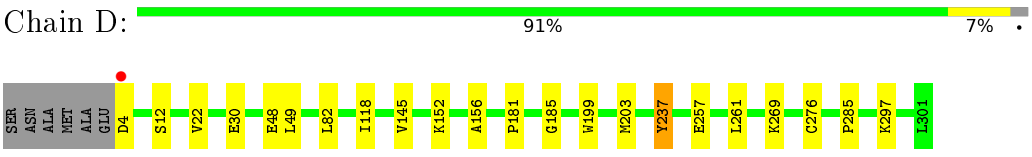
- Molecule 1: N-carbamoylputrescine amidohydrolase

Chain C:



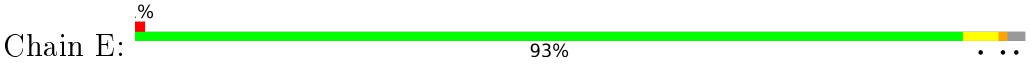
- Molecule 1: N-carbamoylputrescine amidohydrolase

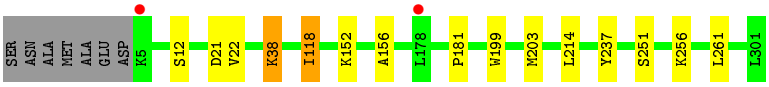
Chain D:



- Molecule 1: N-carbamoylputrescine amidohydrolase

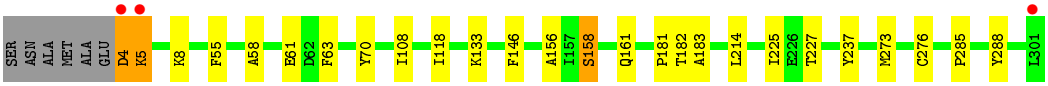
Chain E:





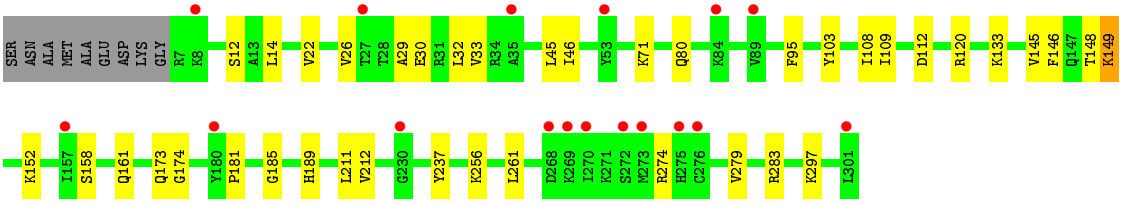
• Molecule 1: N-carbamoylputrescine amidohydrolase

Chain F:



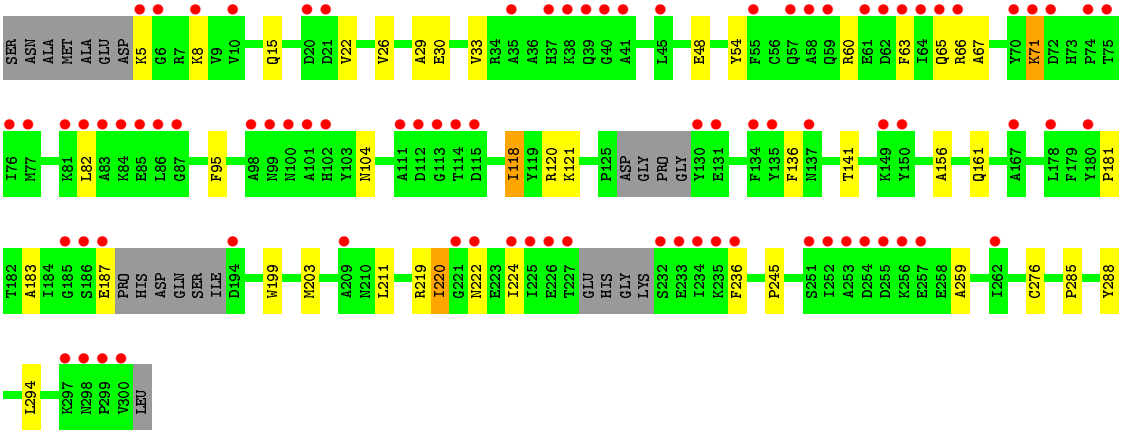
• Molecule 1: N-carbamoylputrescine amidohydrolase

Chain G:



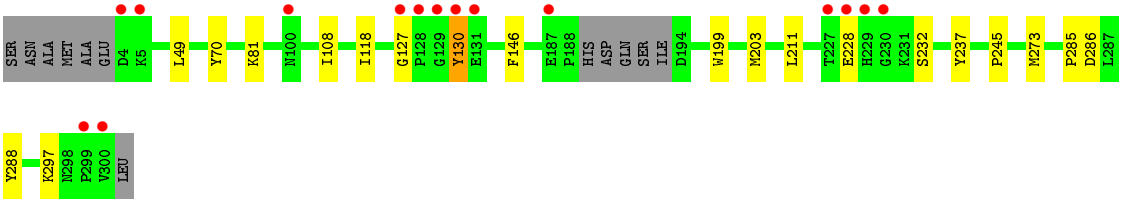
• Molecule 1: N-carbamoylputrescine amidohydrolase

Chain H:



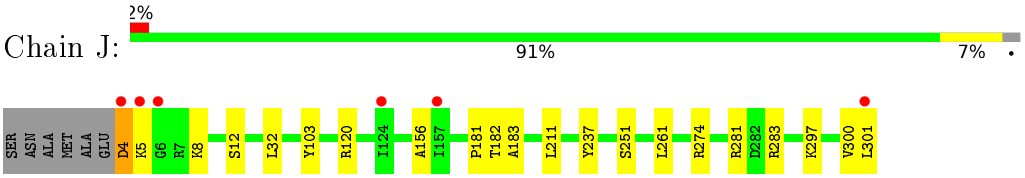
• Molecule 1: N-carbamoylputrescine amidohydrolase

Chain I:



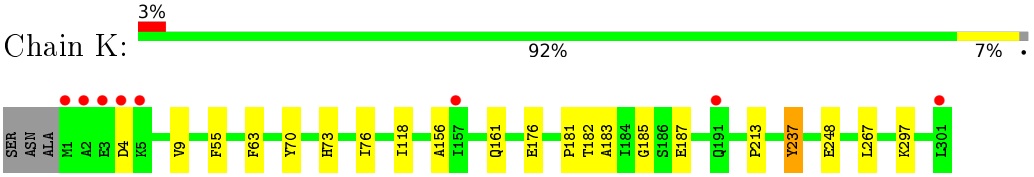
• Molecule 1: N-carbamoylputrescine amidohydrolase

Chain J:



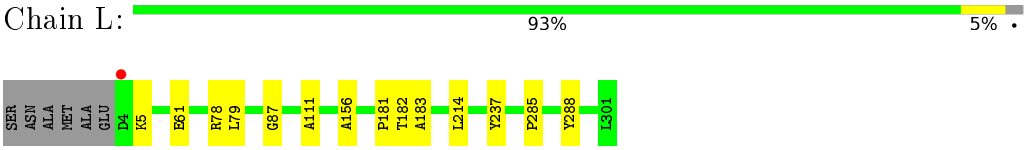
• Molecule 1: N-carbamoylputrescine amidohydrolase

Chain K:



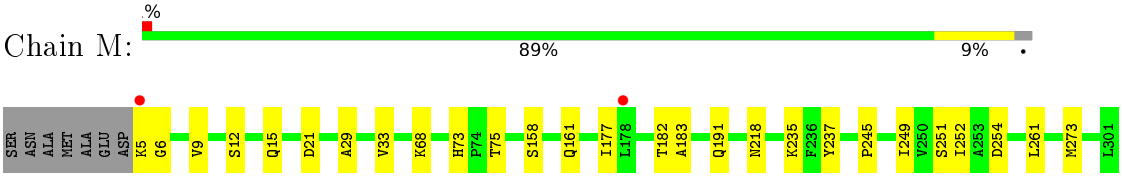
• Molecule 1: N-carbamoylputrescine amidohydrolase

Chain L:



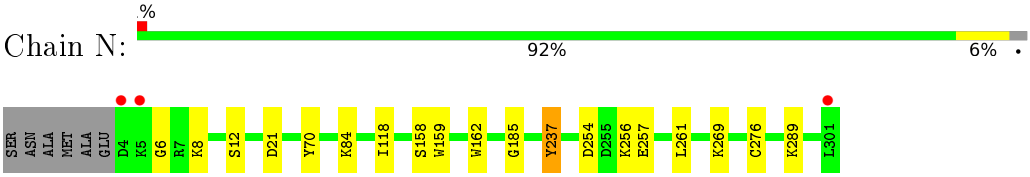
• Molecule 1: N-carbamoylputrescine amidohydrolase

Chain M:



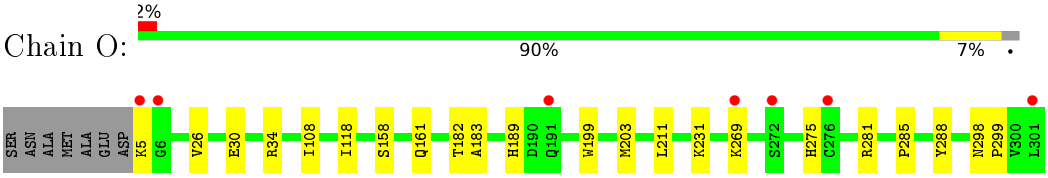
• Molecule 1: N-carbamoylputrescine amidohydrolase

Chain N:



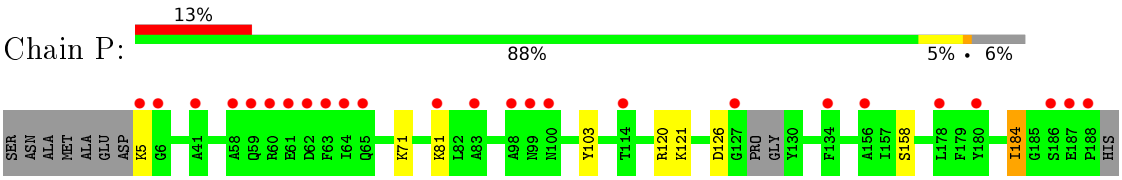
• Molecule 1: N-carbamoylputrescine amidohydrolase

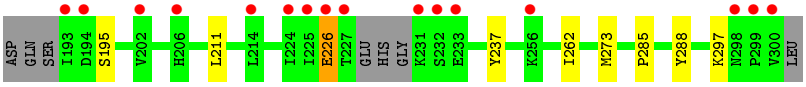
Chain O:



• Molecule 1: N-carbamoylputrescine amidohydrolase

Chain P:




ASP
GLN
SER
I193
D194
S195
V202
H206
L211
L214
I224
I225
E226
T227
GLU
HIS
GLY
K231
S232
E233
Y237
K256
I262
M273
P285
Y288
K297
W298
P299
V300
LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	152.21Å 211.08Å 208.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.53 – 2.29 39.53 – 2.29	Depositor EDS
% Data completeness (in resolution range)	97.5 (39.53-2.29) 97.5 (39.53-2.29)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.154 , 0.206 0.163 , 0.209	Depositor DCC
R_{free} test set	2944 reflections (1.01%)	DCC
Wilson B-factor (Å^2)	28.1	Xtriage
Anisotropy	0.728	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 37.8	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	5 of 294391 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	41665	wwPDB-VP
Average B, all atoms (Å^2)	46.0	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 41.50 % 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 2.3407e-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: PUT, GOL, PEG, EDO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.83	1/2407 (0.0%)	0.81	1/3253 (0.0%)
1	B	0.85	0/2432	0.79	0/3290
1	C	0.88	0/2449	0.81	0/3312
1	D	0.86	1/2434 (0.0%)	0.80	0/3293
1	E	0.81	0/2413	0.78	1/3264 (0.0%)
1	F	0.82	0/2427	0.79	1/3283 (0.0%)
1	G	0.85	0/2400	0.78	0/3248
1	H	0.77	0/2300	0.76	0/3107
1	I	0.84	0/2375	0.79	0/3212
1	J	0.84	0/2427	0.78	0/3283
1	K	0.84	0/2449	0.79	0/3312
1	L	0.86	0/2434	0.79	0/3293
1	M	0.84	0/2426	0.78	0/3282
1	N	0.88	0/2421	0.80	0/3275
1	O	0.79	0/2419	0.77	0/3272
1	P	0.74	0/2337	0.74	0/3157
All	All	0.83	2/38550 (0.0%)	0.79	3/52136 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	130	TYR	CE1-CZ	5.68	1.46	1.38
1	D	257	GLU	CB-CG	5.26	1.62	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	118	ILE	CB-CA-C	-5.24	101.11	111.60
1	F	225	ILE	CB-CA-C	-5.01	101.57	111.60
1	A	225	ILE	CB-CA-C	-5.01	101.58	111.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	2347	0	2321	39	0
1	B	2372	0	2330	15	0
1	C	2390	0	2351	12	0
1	D	2372	0	2337	14	0
1	E	2357	0	2319	11	0
1	F	2368	0	2328	17	0
1	G	2344	0	2303	25	0
1	H	2248	0	2222	27	0
1	I	2318	0	2281	14	0
1	J	2368	0	2328	10	0
1	K	2390	0	2351	12	0
1	L	2372	0	2337	12	0
1	M	2364	0	2333	16	0
1	N	2365	0	2323	12	0
1	O	2360	0	2324	13	0
1	P	2284	0	2260	7	0
2	A	12	0	16	2	0
2	B	12	0	16	1	0
2	C	12	0	16	1	0
2	D	12	0	16	2	0
2	E	24	0	32	0	0
2	F	6	0	8	0	0
2	G	12	0	16	0	0
2	I	6	0	8	0	0
2	J	18	0	24	0	0
2	K	18	0	24	1	0
2	L	6	0	8	4	0
2	M	6	0	8	0	0
2	N	24	0	32	0	0
2	O	6	0	8	0	0
2	P	6	0	8	0	0
3	A	4	0	6	2	0
3	B	8	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	4	0	6	2	0
3	D	8	0	12	1	0
3	F	8	0	12	1	0
3	I	8	0	12	1	0
3	K	4	0	6	1	0
3	L	8	0	12	2	0
3	M	4	0	6	0	0
3	N	4	0	6	0	0
3	P	8	0	12	0	0
4	B	6	0	12	0	0
4	C	6	0	12	0	0
4	D	6	0	12	0	0
4	E	6	0	12	0	0
4	F	6	0	12	0	0
4	G	6	0	12	0	0
4	J	6	0	12	0	0
4	K	6	0	12	1	0
4	L	6	0	12	0	0
4	M	6	0	12	0	0
4	N	6	0	12	0	0
4	O	6	0	12	0	0
5	D	7	0	10	0	0
5	K	7	0	10	0	0
5	L	7	0	10	0	0
6	A	194	0	0	13	0
6	B	264	0	0	3	0
6	C	291	0	0	5	0
6	D	312	0	0	3	0
6	E	274	0	0	5	0
6	F	205	0	0	2	0
6	G	169	0	0	5	0
6	H	61	0	0	2	0
6	I	214	0	0	3	0
6	J	257	0	0	4	0
6	K	270	0	0	4	0
6	L	292	0	0	1	0
6	M	279	0	0	3	0
6	N	291	0	0	5	0
6	O	226	0	0	2	0
6	P	106	0	0	1	0
All	All	41665	0	37564	257	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 3.

All (257) 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:A:65:GLN:HB2	6:A:653:HOH:O	1.70	0.89
1:C:21:ASP:HB2	6:C:740:HOH:O	1.73	0.88
1:N:21:ASP:HB2	6:N:739:HOH:O	1.73	0.86
1:N:269:LYS:HE2	6:N:685:HOH:O	1.79	0.83
1:N:84:LYS:HE2	6:N:660:HOH:O	1.81	0.80
1:G:45:LEU:HD11	1:G:181:PRO:HG3	1.63	0.80
1:F:5:LYS:HE3	1:F:5:LYS:HA	1.64	0.78
1:G:152:LYS:HD2	6:G:622:HOH:O	1.84	0.76
1:A:5:LYS:HD3	6:A:660:HOH:O	1.85	0.75
1:A:59:GLN:NE2	1:A:131:GLU:HG2	2.02	0.74
1:A:130:TYR:CD2	6:A:533:HOH:O	2.44	0.70
1:G:30:GLU:HB3	6:G:504:HOH:O	1.93	0.69
1:H:22:VAL:O	1:H:26:VAL:HG23	1.93	0.68
1:A:5:LYS:HD3	1:A:5:LYS:N	2.09	0.68
6:J:556:HOH:O	3:L:403:EDO:H21	1.94	0.67
1:D:285:PRO:HD2	3:D:404:EDO:H22	1.78	0.66
1:I:273:MET:HE1	6:I:714:HOH:O	1.96	0.66
1:A:78:ARG:HH11	2:A:401:GOL:H12	1.61	0.65
3:A:403:EDO:H21	6:C:615:HOH:O	1.98	0.64
1:A:55:PHE:HB2	1:A:63:PHE:CD2	2.32	0.64
1:A:127:GLY:HA3	6:A:549:HOH:O	1.98	0.63
1:A:203[B]:MET:CE	1:A:216:ALA:HB2	2.29	0.62
6:A:572:HOH:O	1:B:281:ARG:HG2	1.99	0.61
1:O:231:LYS:HE2	6:O:692:HOH:O	2.00	0.61
1:A:199:TRP:CD1	1:A:203[A]:MET:CE	2.83	0.61
1:B:275[A]:HIS:HB2	6:B:686:HOH:O	2.01	0.61
1:G:112:ASP:HB2	6:G:571:HOH:O	2.01	0.60
1:E:256:LYS:HE2	6:E:629:HOH:O	2.00	0.60
1:P:184:ILE:HD11	1:P:195:SER:OG	2.03	0.59
1:A:5:LYS:CD	1:A:5:LYS:N	2.63	0.59
1:C:286:ASP:OD1	3:C:404:EDO:H11	2.03	0.59
1:J:211:LEU:HD12	1:J:274:ARG:HA	1.86	0.58
1:N:269:LYS:CE	6:N:685:HOH:O	2.45	0.58
1:I:130:TYR:HE1	6:I:690:HOH:O	1.85	0.58
1:A:203[B]:MET:HE1	1:A:216:ALA:HB2	1.86	0.58
1:H:95:PHE:CD1	1:H:136:PHE:HE1	2.22	0.58
1:B:156:ALA:O	1:B:181:PRO:HD2	2.04	0.57
1:A:224:ILE:CG2	1:A:231:LYS:HD3	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:301:LEU:HB2	6:J:504:HOH:O	2.05	0.56
1:L:78:ARG:HH11	2:L:402:GOL:H31	1.69	0.56
1:L:5:LYS:HD2	6:L:702:HOH:O	2.06	0.55
1:H:66:ARG:HG3	6:H:452:HOH:O	2.06	0.55
1:E:256:LYS:CE	6:E:629:HOH:O	2.55	0.55
1:H:54:TYR:HB3	1:H:236:PHE:HZ	1.71	0.55
1:L:78:ARG:HD2	2:L:402:GOL:H31	1.89	0.55
1:H:29:ALA:O	1:H:33:VAL:HG23	2.07	0.55
1:A:5:LYS:CE	6:A:660:HOH:O	2.56	0.54
1:H:156:ALA:O	1:H:181:PRO:HD2	2.07	0.54
1:A:199:TRP:CD1	1:A:203[A]:MET:HE2	2.42	0.54
1:A:125:PRO:HG3	6:A:574:HOH:O	2.06	0.54
1:E:12:SER:HA	1:E:261:LEU:O	2.07	0.54
1:P:211:LEU:HD23	1:P:273:MET:HE3	1.90	0.53
1:I:286:ASP:OD1	3:I:402:EDO:H22	2.09	0.52
1:H:15:GLN:NE2	1:H:220:ILE:HD13	2.24	0.52
1:H:71:LYS:HA	1:H:71:LYS:HE3	1.91	0.52
1:K:9:VAL:HG21	1:K:267:LEU:HD11	1.89	0.52
1:F:108:ILE:HG13	1:F:146:PHE:CD2	2.45	0.52
1:A:127:GLY:CA	6:A:549:HOH:O	2.56	0.52
1:A:5:LYS:CD	6:A:660:HOH:O	2.52	0.52
1:M:191:GLN:HG2	1:M:191:GLN:O	2.08	0.52
1:J:156:ALA:O	1:J:181:PRO:HD2	2.09	0.51
1:H:120:ARG:HD2	1:H:141:THR:HG23	1.92	0.51
1:M:9[B]:VAL:HG11	1:M:177:ILE:HD11	1.90	0.51
1:P:285:PRO:HA	1:P:288:TYR:CD2	2.45	0.51
1:M:5:LYS:HD3	1:M:6:GLY:N	2.25	0.51
1:H:60:ARG:NH2	1:H:63:PHE:CE1	2.79	0.51
1:M:29:ALA:O	1:M:33:VAL:HG23	2.10	0.51
1:G:185:GLY:HA2	1:G:237:TYR:CD2	2.46	0.50
1:G:22:VAL:HG23	6:G:574:HOH:O	2.10	0.50
1:D:48:GLU:HG2	1:D:49:LEU:HG	1.93	0.50
1:E:156:ALA:O	1:E:181:PRO:HD2	2.11	0.50
1:E:22:VAL:HG23	6:E:626:HOH:O	2.11	0.50
1:F:61:GLU:HG3	1:H:276[B]:CYS:HB3	1.94	0.50
1:I:81:LYS:HE2	6:I:672:HOH:O	2.12	0.50
1:O:189:HIS:H	1:O:189:HIS:CD2	2.30	0.50
1:B:277:TRP:CZ3	1:B:279:VAL:HG11	2.47	0.50
1:G:108:ILE:HG13	1:G:146:PHE:CD2	2.47	0.50
1:M:68:LYS:HE3	6:M:717:HOH:O	2.11	0.50
1:C:285:PRO:HD2	3:C:404:EDO:H12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:30:GLU:HG3	1:H:82:LEU:HD22	1.93	0.49
1:I:199:TRP:O	1:I:203:MET:HG2	2.12	0.49
1:P:121:LYS:HE3	1:P:158:SER:HB3	1.95	0.49
1:D:156:ALA:O	1:D:181:PRO:HD2	2.11	0.49
1:H:211:LEU:HA	1:H:245:PRO:O	2.13	0.49
1:G:279:VAL:O	1:G:283:ARG:HG3	2.13	0.49
1:G:12:SER:HA	1:G:261:LEU:O	2.12	0.49
1:O:5:LYS:HB3	1:O:5:LYS:NZ	2.28	0.48
1:I:127:GLY:H	1:I:130:TYR:HD2	1.61	0.48
1:N:6:GLY:O	1:N:8:LYS:HE3	2.13	0.48
3:A:403:EDO:C2	6:C:615:HOH:O	2.60	0.48
1:D:185:GLY:HA2	1:D:237:TYR:CD2	2.49	0.48
1:H:285:PRO:HA	1:H:288:TYR:CD2	2.49	0.48
1:A:199:TRP:CD1	1:A:203[A]:MET:HE3	2.49	0.48
1:A:48:GLU:HG2	1:A:49:LEU:HG	1.96	0.48
1:F:58:ALA:HB2	1:F:227:THR:HG22	1.95	0.47
1:A:48:GLU:OE1	1:A:158:SER:HB3	2.14	0.47
1:H:67:ALA:HB2	1:H:95:PHE:CE2	2.49	0.47
1:L:285:PRO:HA	1:L:288:TYR:CD2	2.49	0.47
1:M:21:ASP:HB2	6:M:749:HOH:O	2.14	0.47
1:O:182:THR:HG22	1:O:183:ALA:N	2.29	0.47
1:G:189:HIS:H	1:G:189:HIS:CD2	2.32	0.47
1:K:176:GLU:O	1:K:213:PRO:HD2	2.15	0.47
1:E:199:TRP:CE2	1:E:203:MET:HE1	2.50	0.47
1:A:248:GLU:HB3	6:A:506:HOH:O	2.13	0.47
2:D:401:GOL:H12	6:D:760:HOH:O	2.12	0.47
1:D:12:SER:HA	1:D:261:LEU:O	2.15	0.47
1:E:21:ASP:HB2	6:E:739:HOH:O	2.13	0.47
1:E:214:LEU:HD23	1:E:214:LEU:C	2.35	0.47
1:F:273:MET:HE1	6:F:705:HOH:O	2.14	0.47
1:F:285:PRO:HA	1:F:288:TYR:CD2	2.49	0.47
1:H:199:TRP:O	1:H:203:MET:HG2	2.14	0.46
1:A:12:SER:HA	1:A:261:LEU:O	2.15	0.46
1:G:46:ILE:O	1:G:181:PRO:HB3	2.15	0.46
1:C:78:ARG:HD2	2:C:403:GOL:H31	1.98	0.46
1:E:38:LYS:HA	1:E:38:LYS:CE	2.45	0.46
1:A:78:ARG:HH11	2:A:401:GOL:C1	2.28	0.46
1:N:289:LYS:NZ	6:N:505:HOH:O	2.49	0.46
1:B:12:SER:HA	1:B:261:LEU:O	2.15	0.46
1:B:66:ARG:HB3	2:B:403:GOL:H2	1.98	0.46
2:K:402:GOL:H31	6:K:726:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:ILE:HA	1:A:232:SER:O	2.17	0.45
2:D:403:GOL:H32	6:D:686:HOH:O	2.16	0.45
1:D:199:TRP:CE2	1:D:203:MET:HE1	2.51	0.45
1:A:60:ARG:HB3	1:A:62:ASP:OD1	2.16	0.45
1:G:211:LEU:HD23	1:G:274:ARG:CA	2.47	0.45
1:A:57:GLN:HE22	1:A:132:GLU:HG3	1.81	0.45
1:G:14:LEU:HD22	1:G:32:LEU:HB3	1.98	0.45
1:H:104:ASN:HB3	1:H:121:LYS:HB3	1.98	0.45
1:I:285:PRO:HG2	1:J:300:VAL:HG11	1.99	0.45
1:C:152:LYS:HE2	6:C:552:HOH:O	2.17	0.45
1:M:254:ASP:OD1	1:M:254:ASP:C	2.56	0.44
1:O:30:GLU:O	1:O:34:ARG:HG3	2.17	0.44
1:L:214:LEU:HD23	1:L:214:LEU:C	2.37	0.44
1:A:214:LEU:C	1:A:214:LEU:HD23	2.38	0.44
1:I:211:LEU:HA	1:I:245:PRO:O	2.18	0.44
1:G:29:ALA:HB1	1:G:46:ILE:HD13	1.99	0.44
1:I:228:GLU:H	1:I:228:GLU:CD	2.21	0.44
1:J:12:SER:HA	1:J:261:LEU:O	2.18	0.44
1:K:185:GLY:HA2	1:K:237:TYR:CD2	2.53	0.44
1:K:9:VAL:HG21	1:K:267:LEU:CD1	2.48	0.44
1:N:254:ASP:OD1	1:N:257:GLU:HG2	2.17	0.44
1:C:108:ILE:HG13	1:C:146:PHE:CD2	2.52	0.44
1:M:182:THR:HG22	1:M:183:ALA:N	2.33	0.44
1:F:182:THR:HG22	1:F:183:ALA:N	2.33	0.44
1:H:54:TYR:CE1	1:H:183:ALA:HB3	2.53	0.44
1:F:61:GLU:HG3	1:H:276[A]:CYS:HB2	2.00	0.44
1:I:70:TYR:CZ	1:I:118:ILE:HG23	2.53	0.44
1:L:87:GLY:HA2	1:L:111:ALA:O	2.18	0.44
1:A:43:ILE:HG12	1:A:89:VAL:HB	2.00	0.44
1:C:13:ALA:HB2	1:C:215:VAL:HG13	2.00	0.44
1:O:118:ILE:HG22	6:O:641:HOH:O	2.18	0.44
1:A:5:LYS:HE2	6:A:660:HOH:O	2.16	0.43
1:F:285:PRO:HD2	3:F:403:EDO:H12	1.99	0.43
1:M:245:PRO:CG	1:M:273:MET:HE1	2.48	0.43
1:O:108:ILE:HD13	1:O:108:ILE:N	2.33	0.43
1:D:118:ILE:HD13	1:D:118:ILE:HG21	1.79	0.43
1:D:30:GLU:HG2	1:D:82:LEU:HD22	2.00	0.43
1:G:211:LEU:HD23	1:G:274:ARG:N	2.33	0.43
1:G:80:GLN:HG2	1:G:109:ILE:HD12	2.01	0.43
1:O:298:ASN:HA	1:O:299:PRO:HD2	1.90	0.43
1:N:185:GLY:HA2	1:N:237:TYR:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:103:TYR:CD2	1:J:120:ARG:HD3	2.53	0.43
1:F:70:TYR:CZ	1:F:118:ILE:HG23	2.54	0.43
1:K:161:GLN:HG3	6:K:697:HOH:O	2.19	0.43
1:M:12:SER:HA	1:M:261:LEU:O	2.18	0.43
1:B:266:ASN:ND2	1:B:269:LYS:HE2	2.34	0.43
1:D:145[A]:VAL:CG1	1:D:152:LYS:HG2	2.49	0.43
1:H:161:GLN:HB2	1:H:203:MET:SD	2.58	0.43
1:F:133:LYS:HB3	1:G:133:LYS:HD3	2.01	0.43
1:K:248:GLU:HG2	6:K:526:HOH:O	2.18	0.43
1:K:182:THR:HG22	1:K:183:ALA:N	2.34	0.43
1:H:104:ASN:HB3	1:H:121:LYS:CB	2.48	0.43
1:I:286:ASP:N	1:I:286:ASP:OD1	2.49	0.43
1:J:283:ARG:HD3	6:J:531:HOH:O	2.19	0.43
1:P:226:GLU:HB3	6:P:589:HOH:O	2.18	0.43
1:A:228:GLU:H	1:A:228:GLU:CD	2.23	0.42
1:K:156:ALA:O	1:K:181:PRO:HD2	2.20	0.42
1:M:235:LYS:HE2	6:M:583:HOH:O	2.19	0.42
1:D:297:LYS:HE2	1:D:297:LYS:HB3	1.78	0.42
1:D:4:ASP:OD1	1:D:269:LYS:NZ	2.51	0.42
1:I:285:PRO:HA	1:I:288:TYR:CD2	2.55	0.42
1:J:182:THR:HG22	1:J:183:ALA:N	2.33	0.42
1:M:245:PRO:HG2	1:M:273:MET:CE	2.49	0.42
1:B:108:ILE:N	1:B:108:ILE:HD12	2.35	0.42
1:F:161:GLN:OE1	6:F:501:HOH:O	2.21	0.42
1:K:187:GLU:OE2	4:K:401:PUT:N2	2.53	0.42
1:A:108:ILE:HG13	1:A:146:PHE:CD1	2.54	0.42
1:B:14:LEU:HD22	1:B:32:LEU:HB3	2.02	0.42
6:A:564:HOH:O	3:B:405:EDO:H11	2.19	0.42
1:C:156:ALA:O	1:C:181:PRO:HD2	2.19	0.42
1:D:22:VAL:HG23	6:D:621:HOH:O	2.19	0.42
1:O:199:TRP:CE2	1:O:203:MET:HE1	2.55	0.42
1:O:275:HIS:O	1:O:281:ARG:NH2	2.52	0.42
1:A:298:ASN:HA	1:A:299:PRO:HD3	1.94	0.42
1:A:147:GLN:OE1	1:A:152:LYS:HE2	2.20	0.42
1:K:55:PHE:HB2	1:K:63:PHE:CD2	2.55	0.42
1:L:78:ARG:CD	2:L:402:GOL:H31	2.50	0.42
1:L:79:LEU:HA	1:L:79:LEU:HD23	1.83	0.42
1:F:156:ALA:O	1:F:181:PRO:HD2	2.20	0.42
1:F:55:PHE:HB2	1:F:63:PHE:CD2	2.54	0.42
1:G:145:VAL:HG21	1:G:173:GLN:O	2.20	0.42
1:L:61:GLU:HB2	1:N:276:CYS:SG	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:103:TYR:CG	1:P:120:ARG:HD3	2.55	0.42
1:B:275[B]:HIS:HB2	6:B:686:HOH:O	2.21	0.41
1:F:4:ASP:O	1:F:8:LYS:CE	2.68	0.41
1:H:66:ARG:CG	6:H:452:HOH:O	2.66	0.41
1:M:15:GLN:HG3	1:M:218:ASN:O	2.19	0.41
1:O:211:LEU:HD12	1:O:211:LEU:HA	1.92	0.41
1:G:29:ALA:O	1:G:33:VAL:HG23	2.19	0.41
1:I:49:LEU:HA	1:I:49:LEU:HD23	1.88	0.41
1:M:249:ILE:HG21	1:M:252:ILE:HB	2.02	0.41
1:C:285:PRO:HA	1:C:288:TYR:CD2	2.54	0.41
1:J:32:LEU:HD23	1:J:32:LEU:HA	1.89	0.41
1:K:73:HIS:HB3	1:K:76:ILE:HD12	2.02	0.41
1:A:125:PRO:HB2	1:A:130:TYR:CB	2.50	0.41
1:C:22:VAL:HG23	6:C:714:HOH:O	2.20	0.41
1:C:185:GLY:HA2	1:C:237:TYR:CD2	2.56	0.41
1:H:118:ILE:HD12	1:H:118:ILE:H	1.85	0.41
1:H:15:GLN:HB3	1:H:259:ALA:HB3	2.01	0.41
3:K:405:EDO:H21	6:K:632:HOH:O	2.19	0.41
1:M:245:PRO:HB2	1:M:273:MET:CE	2.51	0.41
1:F:214:LEU:C	1:F:214:LEU:HD23	2.41	0.41
1:K:70:TYR:CZ	1:K:118:ILE:HG23	2.56	0.41
1:A:224:ILE:HG23	1:A:231:LYS:HD3	2.01	0.41
1:B:78:ARG:NE	6:B:502:HOH:O	2.45	0.41
1:E:118:ILE:HG21	1:E:118:ILE:HD13	1.80	0.41
1:G:80:GLN:CG	1:G:109:ILE:HD12	2.51	0.41
1:H:48:GLU:O	1:H:219:ARG:NH2	2.47	0.41
1:N:70:TYR:CZ	1:N:118:ILE:HG23	2.56	0.41
1:P:262:ILE:HD13	1:P:262:ILE:HA	1.85	0.41
1:A:187:GLU:HG2	6:A:670:HOH:O	2.21	0.41
1:A:22:VAL:O	1:A:26:VAL:HG23	2.21	0.41
1:B:87:GLY:HA2	1:B:111:ALA:O	2.21	0.41
1:C:12:SER:HA	1:C:261:LEU:O	2.20	0.41
1:H:67:ALA:HB2	1:H:95:PHE:CZ	2.56	0.41
1:B:61:GLU:HG3	1:D:276[A]:CYS:HB2	2.03	0.41
1:G:103:TYR:CE2	1:G:120:ARG:CZ	3.04	0.41
6:J:556:HOH:O	3:L:403:EDO:C2	2.62	0.41
1:O:26:VAL:O	1:O:30:GLU:HG3	2.21	0.41
1:A:92:VAL:C	1:A:106:ILE:HG13	2.41	0.41
1:G:174:GLY:HA3	6:G:510:HOH:O	2.21	0.41
1:F:133:LYS:CD	1:G:133:LYS:HB3	2.51	0.40
1:J:4:ASP:HB3	1:J:8:LYS:HE2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:182:THR:HG22	1:L:183:ALA:N	2.36	0.40
1:M:73:HIS:CE1	1:M:75:THR:HB	2.56	0.40
1:B:82:LEU:HA	1:B:82:LEU:HD12	1.88	0.40
1:G:22:VAL:O	1:G:26:VAL:HG23	2.21	0.40
1:H:65:GLN:HA	1:H:65:GLN:OE1	2.22	0.40
1:L:156:ALA:O	1:L:181:PRO:HD2	2.20	0.40
1:N:12:SER:HA	1:N:261:LEU:O	2.22	0.40
1:I:108:ILE:HG13	1:I:146:PHE:CD2	2.57	0.40
1:L:78:ARG:HH11	2:L:402:GOL:C3	2.33	0.40
1:N:159:TRP:CE3	1:N:162:TRP:CD1	3.09	0.40
1:O:285:PRO:HA	1:O:288:TYR:CD2	2.57	0.40
1:B:61:GLU:HG3	1:D:276[B]:CYS:HB3	2.04	0.40
1:E:152:LYS:HE2	6:E:522:HOH:O	2.20	0.40
1:G:148:THR:O	1:G:149:LYS:C	2.60	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	293/304 (96%)	278 (95%)	14 (5%)	1 (0%)	46	57
1	B	297/304 (98%)	285 (96%)	11 (4%)	1 (0%)	46	57
1	C	300/304 (99%)	291 (97%)	9 (3%)	0	100	100
1	D	298/304 (98%)	290 (97%)	8 (3%)	0	100	100
1	E	295/304 (97%)	285 (97%)	10 (3%)	0	100	100
1	F	297/304 (98%)	284 (96%)	12 (4%)	1 (0%)	46	57
1	G	293/304 (96%)	281 (96%)	11 (4%)	1 (0%)	46	57
1	H	275/304 (90%)	254 (92%)	21 (8%)	0	100	100
1	I	289/304 (95%)	277 (96%)	12 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	J	297/304 (98%)	286 (96%)	11 (4%)	0	100 100
1	K	300/304 (99%)	291 (97%)	9 (3%)	0	100 100
1	L	298/304 (98%)	290 (97%)	8 (3%)	0	100 100
1	M	297/304 (98%)	286 (96%)	10 (3%)	1 (0%)	46 57
1	N	296/304 (97%)	286 (97%)	9 (3%)	1 (0%)	46 57
1	O	296/304 (97%)	285 (96%)	10 (3%)	1 (0%)	46 57
1	P	280/304 (92%)	271 (97%)	9 (3%)	0	100 100
All	All	4701/4864 (97%)	4520 (96%)	174 (4%)	7 (0%)	56 68

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	158	SER
1	A	158	SER
1	N	158	SER
1	F	158	SER
1	M	158	SER
1	O	158	SER
1	B	158	SER

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	247/252 (98%)	234 (95%)	13 (5%)	28 37
1	B	249/252 (99%)	244 (98%)	5 (2%)	63 79
1	C	251/252 (100%)	247 (98%)	4 (2%)	70 84
1	D	250/252 (99%)	249 (100%)	1 (0%)	93 97
1	E	247/252 (98%)	244 (99%)	3 (1%)	78 89
1	F	249/252 (99%)	243 (98%)	6 (2%)	57 74
1	G	246/252 (98%)	239 (97%)	7 (3%)	51 68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	H	236/252 (94%)	227 (96%)	9 (4%)	40 54
1	I	243/252 (96%)	239 (98%)	4 (2%)	70 84
1	J	249/252 (99%)	243 (98%)	6 (2%)	57 74
1	K	251/252 (100%)	248 (99%)	3 (1%)	78 89
1	L	250/252 (99%)	249 (100%)	1 (0%)	93 97
1	M	249/252 (99%)	246 (99%)	3 (1%)	78 89
1	N	248/252 (98%)	246 (99%)	2 (1%)	86 94
1	O	248/252 (98%)	246 (99%)	2 (1%)	86 94
1	P	240/252 (95%)	232 (97%)	8 (3%)	45 61
All	All	3953/4032 (98%)	3876 (98%)	77 (2%)	65 81

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	23	SER
1	A	64	ILE
1	A	65	GLN
1	A	100	ASN
1	A	130	TYR
1	A	131	GLU
1	A	203[A]	MET
1	A	203[B]	MET
1	A	231	LYS
1	A	237	TYR
1	A	251	SER
1	A	297	LYS
1	B	161	GLN
1	B	237	TYR
1	B	251	SER
1	B	272	SER
1	B	297	LYS
1	C	3	GLU
1	C	4	ASP
1	C	5	LYS
1	C	237	TYR
1	D	237	TYR
1	E	38	LYS
1	E	237	TYR

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Mol	Chain	Res	Type
1	E	251	SER
1	F	4	ASP
1	F	5	LYS
1	F	158	SER
1	F	237	TYR
1	F	276[A]	CYS
1	F	276[B]	CYS
1	G	71	LYS
1	G	95	PHE
1	G	149	LYS
1	G	161	GLN
1	G	212	VAL
1	G	256	LYS
1	G	297	LYS
1	H	5	LYS
1	H	8	LYS
1	H	71	LYS
1	H	118	ILE
1	H	187	GLU
1	H	220	ILE
1	H	222	ASN
1	H	224	ILE
1	H	294	LEU
1	I	130	TYR
1	I	232	SER
1	I	237	TYR
1	I	297	LYS
1	J	4	ASP
1	J	5	LYS
1	J	237	TYR
1	J	251	SER
1	J	281	ARG
1	J	297	LYS
1	K	4	ASP
1	K	237	TYR
1	K	297	LYS
1	L	237	TYR
1	M	161	GLN
1	M	237	TYR
1	M	251	SER
1	N	237	TYR
1	N	256	LYS

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Mol	Chain	Res	Type
1	O	161	GLN
1	O	269	LYS
1	P	5	LYS
1	P	71	LYS
1	P	81	LYS
1	P	126	ASP
1	P	184	ILE
1	P	226	GLU
1	P	237	TYR
1	P	297	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	100	ASN
1	A	161	GLN
1	B	65	GLN
1	C	65	GLN
1	C	191	GLN
1	D	204	GLN
1	E	65	GLN
1	F	65	GLN
1	G	65	GLN
1	G	102	HIS
1	G	189	HIS
1	H	161	GLN
1	H	222	ASN
1	I	161	GLN
1	J	65	GLN
1	K	65	GLN
1	L	65	GLN
1	M	65	GLN
1	N	65	GLN
1	O	65	GLN
1	O	102	HIS
1	O	189	HIS
1	P	57	GLN
1	P	99	ASN
1	P	100	ASN
1	P	161	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

62 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GOL	A	401	-	5,5,5	0.55	0	5,5,5	0.62	0
2	GOL	A	402	-	5,5,5	0.43	0	5,5,5	0.30	0
3	EDO	A	403	-	3,3,3	0.50	0	2,2,2	0.38	0
4	PUT	B	401	-	5,5,5	0.36	0	4,4,4	0.95	0
2	GOL	B	402	-	5,5,5	0.64	0	5,5,5	0.62	0
2	GOL	B	403	-	5,5,5	0.29	0	5,5,5	0.34	0
3	EDO	B	404	-	3,3,3	0.58	0	2,2,2	0.20	0
3	EDO	B	405	-	3,3,3	0.66	0	2,2,2	0.07	0
4	PUT	C	401	-	5,5,5	0.28	0	4,4,4	1.33	1 (25%)
2	GOL	C	402	-	5,5,5	0.40	0	5,5,5	0.42	0
2	GOL	C	403	-	5,5,5	0.47	0	5,5,5	0.41	0
3	EDO	C	404	-	3,3,3	0.68	0	2,2,2	0.40	0
2	GOL	D	401	-	5,5,5	0.37	0	5,5,5	0.33	0
4	PUT	D	402	-	5,5,5	0.22	0	4,4,4	1.15	1 (25%)
2	GOL	D	403	-	5,5,5	0.75	0	5,5,5	0.53	0
3	EDO	D	404	-	3,3,3	0.60	0	2,2,2	0.25	0
3	EDO	D	405	-	3,3,3	0.49	0	2,2,2	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	PEG	D	406	-	6,6,6	0.70	0	5,5,5	0.17	0
4	PUT	E	401	-	5,5,5	0.20	0	4,4,4	1.18	1 (25%)
2	GOL	E	402	-	5,5,5	0.33	0	5,5,5	0.39	0
2	GOL	E	403	-	5,5,5	0.44	0	5,5,5	0.48	0
2	GOL	E	404	-	5,5,5	0.32	0	5,5,5	0.27	0
2	GOL	E	405	-	5,5,5	0.54	0	5,5,5	0.45	0
4	PUT	F	401	-	5,5,5	0.40	0	4,4,4	0.63	0
2	GOL	F	402	-	5,5,5	0.46	0	5,5,5	0.25	0
3	EDO	F	403	-	3,3,3	0.59	0	2,2,2	0.24	0
3	EDO	F	404	-	3,3,3	0.57	0	2,2,2	0.35	0
4	PUT	G	401	-	5,5,5	0.24	0	4,4,4	1.56	1 (25%)
2	GOL	G	402	-	5,5,5	0.40	0	5,5,5	0.59	0
2	GOL	G	403	-	5,5,5	0.42	0	5,5,5	0.25	0
2	GOL	I	401	-	5,5,5	0.42	0	5,5,5	0.23	0
3	EDO	I	402	-	3,3,3	0.63	0	2,2,2	0.10	0
3	EDO	I	403	-	3,3,3	0.49	0	2,2,2	0.50	0
4	PUT	J	401	-	5,5,5	0.42	0	4,4,4	1.39	1 (25%)
2	GOL	J	402	-	5,5,5	0.34	0	5,5,5	0.43	0
2	GOL	J	403	-	5,5,5	0.54	0	5,5,5	0.69	0
2	GOL	J	404	-	5,5,5	0.29	0	5,5,5	0.30	0
4	PUT	K	401	-	5,5,5	0.42	0	4,4,4	0.90	0
2	GOL	K	402	-	5,5,5	0.57	0	5,5,5	0.37	0
2	GOL	K	403	-	5,5,5	0.61	0	5,5,5	0.44	0
2	GOL	K	404	-	5,5,5	0.48	0	5,5,5	0.30	0
3	EDO	K	405	-	3,3,3	0.58	0	2,2,2	0.16	0
5	PEG	K	406	-	6,6,6	0.61	0	5,5,5	0.15	0
4	PUT	L	401	-	5,5,5	0.45	0	4,4,4	1.13	1 (25%)
2	GOL	L	402	-	5,5,5	0.74	0	5,5,5	0.53	0
3	EDO	L	403	-	3,3,3	0.52	0	2,2,2	0.30	0
3	EDO	L	404	-	3,3,3	0.53	0	2,2,2	0.16	0
5	PEG	L	405	-	6,6,6	0.60	0	5,5,5	0.35	0
4	PUT	M	401	-	5,5,5	0.51	0	4,4,4	0.91	0
2	GOL	M	402	-	5,5,5	0.35	0	5,5,5	0.20	0
3	EDO	M	403	-	3,3,3	0.75	0	2,2,2	0.10	0
2	GOL	N	401	-	5,5,5	0.19	0	5,5,5	0.24	0
4	PUT	N	402	-	5,5,5	0.30	0	4,4,4	0.72	0
2	GOL	N	403	-	5,5,5	0.74	0	5,5,5	0.66	0
2	GOL	N	404	-	5,5,5	0.41	0	5,5,5	0.28	0
2	GOL	N	405	-	5,5,5	0.61	0	5,5,5	0.54	0
3	EDO	N	406	-	3,3,3	0.58	0	2,2,2	0.03	0
4	PUT	O	401	-	5,5,5	0.39	0	4,4,4	1.15	1 (25%)
2	GOL	O	402	-	5,5,5	0.24	0	5,5,5	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GOL	P	401	-	5,5,5	0.39	0	5,5,5	0.18	0
3	EDO	P	402	-	3,3,3	0.58	0	2,2,2	0.27	0
3	EDO	P	403	-	3,3,3	0.51	0	2,2,2	0.36	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
3	EDO	A	403	-	-	0/1/1/1	0/0/0/0
4	PUT	B	401	-	-	0/3/3/3	0/0/0/0
2	GOL	B	402	-	-	0/4/4/4	0/0/0/0
2	GOL	B	403	-	-	0/4/4/4	0/0/0/0
3	EDO	B	404	-	-	0/1/1/1	0/0/0/0
3	EDO	B	405	-	-	0/1/1/1	0/0/0/0
4	PUT	C	401	-	-	0/3/3/3	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
3	EDO	C	404	-	-	0/1/1/1	0/0/0/0
2	GOL	D	401	-	-	0/4/4/4	0/0/0/0
4	PUT	D	402	-	-	0/3/3/3	0/0/0/0
2	GOL	D	403	-	-	0/4/4/4	0/0/0/0
3	EDO	D	404	-	-	0/1/1/1	0/0/0/0
3	EDO	D	405	-	-	0/1/1/1	0/0/0/0
5	PEG	D	406	-	-	0/4/4/4	0/0/0/0
4	PUT	E	401	-	-	0/3/3/3	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
4	PUT	F	401	-	-	0/3/3/3	0/0/0/0
2	GOL	F	402	-	-	0/4/4/4	0/0/0/0
3	EDO	F	403	-	-	0/1/1/1	0/0/0/0
3	EDO	F	404	-	-	0/1/1/1	0/0/0/0
4	PUT	G	401	-	-	0/3/3/3	0/0/0/0
2	GOL	G	402	-	-	0/4/4/4	0/0/0/0
2	GOL	G	403	-	-	0/4/4/4	0/0/0/0
2	GOL	I	401	-	-	0/4/4/4	0/0/0/0
3	EDO	I	402	-	-	0/1/1/1	0/0/0/0
3	EDO	I	403	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PUT	J	401	-	-	0/3/3/3	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
4	PUT	K	401	-	-	0/3/3/3	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
3	EDO	K	405	-	-	0/1/1/1	0/0/0/0
5	PEG	K	406	-	-	0/4/4/4	0/0/0/0
4	PUT	L	401	-	-	0/3/3/3	0/0/0/0
2	GOL	L	402	-	-	0/4/4/4	0/0/0/0
3	EDO	L	403	-	-	0/1/1/1	0/0/0/0
3	EDO	L	404	-	-	0/1/1/1	0/0/0/0
5	PEG	L	405	-	-	0/4/4/4	0/0/0/0
4	PUT	M	401	-	-	0/3/3/3	0/0/0/0
2	GOL	M	402	-	-	0/4/4/4	0/0/0/0
3	EDO	M	403	-	-	0/1/1/1	0/0/0/0
2	GOL	N	401	-	-	0/4/4/4	0/0/0/0
4	PUT	N	402	-	-	0/3/3/3	0/0/0/0
2	GOL	N	403	-	-	0/4/4/4	0/0/0/0
2	GOL	N	404	-	-	0/4/4/4	0/0/0/0
2	GOL	N	405	-	-	0/4/4/4	0/0/0/0
3	EDO	N	406	-	-	0/1/1/1	0/0/0/0
4	PUT	O	401	-	-	0/3/3/3	0/0/0/0
2	GOL	O	402	-	-	0/4/4/4	0/0/0/0
2	GOL	P	401	-	-	0/4/4/4	0/0/0/0
3	EDO	P	402	-	-	0/1/1/1	0/0/0/0
3	EDO	P	403	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	401	PUT	C2-C3-C4	-2.98	99.39	113.89
4	C	401	PUT	C2-C3-C4	-2.63	101.12	113.89
4	J	401	PUT	C2-C3-C4	-2.57	101.38	113.89
4	L	401	PUT	C2-C3-C4	-2.23	103.05	113.89
4	E	401	PUT	C2-C3-C4	-2.23	103.06	113.89
4	O	401	PUT	C2-C3-C4	-2.19	103.22	113.89
4	D	402	PUT	C2-C3-C4	-2.14	103.51	113.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	GOL	2	0
3	A	403	EDO	2	0
2	B	403	GOL	1	0
3	B	405	EDO	1	0
2	C	403	GOL	1	0
3	C	404	EDO	2	0
2	D	401	GOL	1	0
2	D	403	GOL	1	0
3	D	404	EDO	1	0
3	F	403	EDO	1	0
3	I	402	EDO	1	0
4	K	401	PUT	1	0
2	K	402	GOL	1	0
3	K	405	EDO	1	0
2	L	402	GOL	4	0
3	L	403	EDO	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, 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	295/304 (97%)	-0.01	22 (7%) 17 24	28, 45, 95, 132	0
1	B	298/304 (98%)	-0.20	7 (2%) 64 72	25, 36, 59, 115	0
1	C	301/304 (99%)	-0.34	4 (1%) 79 84	25, 35, 54, 112	0
1	D	298/304 (98%)	-0.43	1 (0%) 94 96	24, 33, 49, 92	0
1	E	297/304 (97%)	-0.33	2 (0%) 89 92	26, 37, 57, 92	0
1	F	298/304 (98%)	-0.40	3 (1%) 84 88	28, 44, 64, 93	0
1	G	295/304 (97%)	0.44	17 (5%) 26 35	47, 65, 84, 101	0
1	H	282/304 (92%)	1.45	85 (30%) 1 1	50, 85, 118, 136	0
1	I	292/304 (96%)	-0.15	15 (5%) 32 41	28, 41, 84, 138	0
1	J	298/304 (98%)	-0.26	6 (2%) 68 75	26, 36, 58, 118	0
1	K	301/304 (99%)	-0.27	8 (2%) 58 67	26, 37, 59, 111	0
1	L	298/304 (98%)	-0.48	1 (0%) 94 96	24, 34, 50, 91	0
1	M	297/304 (97%)	-0.33	2 (0%) 89 92	25, 35, 52, 88	0
1	N	298/304 (98%)	-0.47	3 (1%) 84 88	25, 35, 52, 92	0
1	O	297/304 (97%)	-0.20	7 (2%) 62 71	32, 46, 66, 108	0
1	P	287/304 (94%)	0.69	41 (14%) 4 6	34, 61, 104, 119	0
All	All	4732/4864 (97%)	-0.09	224 (4%) 35 44	24, 40, 87, 138	0

All (224) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	300	VAL	7.3
1	H	58	ALA	7.3
1	J	4	ASP	6.9
1	B	4	ASP	6.3
1	A	230	GLY	6.2

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Mol	Chain	Res	Type	RSRZ
1	I	229	HIS	6.2
1	H	77	MET	6.1
1	A	128	PRO	5.9
1	H	232	SER	5.9
1	H	186	SER	5.8
1	P	227	THR	5.8
1	P	100	ASN	5.6
1	H	227	THR	5.6
1	P	63	PHE	5.4
1	I	230	GLY	5.4
1	A	301	LEU	5.4
1	H	99	ASN	5.3
1	I	4	ASP	5.3
1	A	193	ILE	5.3
1	A	229	HIS	5.1
1	H	234	ILE	5.1
1	P	193	ILE	5.0
1	P	58	ALA	4.9
1	O	5	LYS	4.8
1	H	185	GLY	4.7
1	B	5	LYS	4.6
1	I	227	THR	4.6
1	H	21	ASP	4.6
1	P	232	SER	4.5
1	H	61	GLU	4.5
1	H	257	GLU	4.4
1	P	61	GLU	4.4
1	H	111	ALA	4.4
1	I	228	GLU	4.4
1	H	100	ASN	4.3
1	G	273	MET	4.3
1	A	228	GLU	4.3
1	K	1	MET	4.2
1	H	225	ILE	4.2
1	A	130	TYR	4.2
1	F	4	ASP	4.2
1	H	134	PHE	4.2
1	H	298	ASN	4.2
1	A	192	SER	4.2
1	H	256	LYS	4.2
1	P	5	LYS	4.2
1	H	233	GLU	4.1

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Mol	Chain	Res	Type	RSRZ
1	H	224	ILE	4.1
1	P	300	VAL	4.1
1	K	4	ASP	4.1
1	H	59	GLN	4.1
1	H	72	ASP	4.0
1	H	137	ASN	4.0
1	G	276	CYS	4.0
1	A	127	GLY	4.0
1	H	81	LYS	4.0
1	C	3	GLU	3.9
1	C	2	ALA	3.9
1	H	221	GLY	3.9
1	K	3	GLU	3.8
1	I	128	PRO	3.8
1	H	102	HIS	3.8
1	A	227	THR	3.8
1	H	74	PRO	3.8
1	H	85	GLU	3.8
1	J	5	LYS	3.8
1	H	65	GLN	3.7
1	H	299	PRO	3.7
1	H	178	LEU	3.7
1	P	298	ASN	3.7
1	P	188	PRO	3.7
1	P	65	GLN	3.7
1	O	6	GLY	3.6
1	D	4	ASP	3.6
1	H	112	ASP	3.6
1	F	5	LYS	3.6
1	P	256	LYS	3.6
1	H	226	GLU	3.6
1	H	253	ALA	3.6
1	P	134	PHE	3.6
1	P	225	ILE	3.6
1	H	6	GLY	3.6
1	A	299	PRO	3.6
1	P	99	ASN	3.5
1	P	226	GLU	3.5
1	H	180	TYR	3.5
1	P	231	LYS	3.4
1	H	187	GLU	3.4
1	I	130	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
1	H	62	ASP	3.4
1	H	75	THR	3.4
1	P	187	GLU	3.4
1	H	86	LEU	3.4
1	H	87	GLY	3.4
1	H	194	ASP	3.4
1	H	254	ASP	3.4
1	P	98	ALA	3.4
1	H	40	GLY	3.3
1	L	4	ASP	3.3
1	H	222	ASN	3.3
1	A	126	ASP	3.3
1	H	98	ALA	3.3
1	H	8	LYS	3.3
1	J	6	GLY	3.3
1	A	226	GLU	3.3
1	A	188	PRO	3.3
1	H	114	THR	3.3
1	I	129	GLY	3.2
1	H	63	PHE	3.2
1	K	2	ALA	3.2
1	H	83	ALA	3.2
1	H	66	ARG	3.2
1	H	38	LYS	3.2
1	A	191	GLN	3.2
1	H	57	GLN	3.1
1	G	272	SER	3.1
1	P	62	ASP	3.1
1	P	178	LEU	3.1
1	H	135	TYR	3.0
1	P	299	PRO	3.0
1	A	133	LYS	3.0
1	H	131	GLU	3.0
1	H	255	ASP	3.0
1	E	5	LYS	3.0
1	G	35	ALA	2.9
1	H	236	PHE	2.9
1	F	301	LEU	2.9
1	C	4	ASP	2.9
1	O	276[A]	CYS	2.9
1	H	130	TYR	2.9
1	P	127	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	P	224	ILE	2.9
1	H	20	ASP	2.9
1	H	82	LEU	2.9
1	P	156	ALA	2.9
1	I	299	PRO	2.9
1	N	4	ASP	2.8
1	H	167	ALA	2.8
1	G	268	ASP	2.8
1	C	1	MET	2.8
1	H	150	TYR	2.8
1	P	59	GLN	2.8
1	P	186	SER	2.8
1	H	41	ALA	2.7
1	H	113	GLY	2.7
1	A	300	VAL	2.7
1	B	6	GLY	2.7
1	A	61	GLU	2.7
1	I	100	ASN	2.7
1	H	297	LYS	2.7
1	H	84	LYS	2.7
1	H	235	LYS	2.7
1	H	71	LYS	2.6
1	H	101	ALA	2.6
1	N	301	LEU	2.6
1	H	35	ALA	2.6
1	H	209	ALA	2.6
1	H	76	ILE	2.6
1	P	6	GLY	2.6
1	G	301	LEU	2.6
1	H	149	LYS	2.6
1	P	233	GLU	2.5
1	G	84	LYS	2.5
1	P	180	TYR	2.5
1	B	157	ILE	2.5
1	G	270	ILE	2.5
1	P	194	ASP	2.5
1	P	214	LEU	2.5
1	H	115	ASP	2.5
1	G	89	VAL	2.4
1	G	27	THR	2.4
1	H	64	ILE	2.4
1	H	45	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	39	GLN	2.4
1	G	157	ILE	2.4
1	H	37	HIS	2.4
1	I	131	GLU	2.4
1	M	5	LYS	2.4
1	P	114	THR	2.4
1	H	5	LYS	2.3
1	P	202	VAL	2.3
1	P	60	ARG	2.3
1	O	191	GLN	2.3
1	J	157	ILE	2.3
1	I	127	GLY	2.3
1	H	251	SER	2.3
1	O	272	SER	2.3
1	G	8	LYS	2.3
1	J	301	LEU	2.3
1	G	53	TYR	2.3
1	B	215	VAL	2.3
1	A	231	LYS	2.3
1	H	262	ILE	2.3
1	K	5	LYS	2.2
1	O	269	LYS	2.2
1	M	178	LEU	2.2
1	A	298	ASN	2.2
1	K	191	GLN	2.2
1	J	124	ILE	2.2
1	G	269	LYS	2.2
1	I	300	VAL	2.2
1	A	131	GLU	2.2
1	N	5	LYS	2.2
1	H	70	TYR	2.2
1	G	275	HIS	2.2
1	H	252	ILE	2.2
1	A	5	LYS	2.2
1	P	41	ALA	2.2
1	E	178	LEU	2.2
1	G	230	GLY	2.1
1	G	180	TYR	2.1
1	I	187	GLU	2.1
1	I	5	LYS	2.1
1	P	64	ILE	2.1
1	B	203	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	P	83	ALA	2.1
1	K	157	ILE	2.1
1	P	81	LYS	2.1
1	P	206	HIS	2.1
1	O	301	LEU	2.0
1	H	10	VAL	2.0
1	H	55	PHE	2.0
1	B	180	TYR	2.0
1	K	301	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
2	GOL	N	405	6/6	0.78	0.29	9.84	62,69,85,89	0
4	PUT	G	401	6/6	0.89	0.39	9.71	66,68,72,76	0
5	PEG	L	405	7/7	0.83	0.38	9.25	62,68,83,83	0
4	PUT	F	401	6/6	0.94	0.32	9.20	59,62,67,67	0
2	GOL	E	404	6/6	0.94	0.22	9.04	49,54,60,61	0
4	PUT	N	402	6/6	0.96	0.36	9.00	47,47,49,51	0
2	GOL	A	401	6/6	0.83	0.19	8.02	55,74,75,75	0
2	GOL	D	403	6/6	0.87	0.40	7.58	48,60,69,72	0
2	GOL	I	401	6/6	0.92	0.15	7.12	54,60,69,70	0
2	GOL	K	404	6/6	0.92	0.28	6.41	53,58,64,71	0
2	GOL	J	403	6/6	0.84	0.23	6.18	62,64,74,80	0
4	PUT	O	401	6/6	0.95	0.29	6.07	47,48,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	PUT	M	401	6/6	0.96	0.32	5.98	34,35,37,39	0
4	PUT	L	401	6/6	0.97	0.32	5.71	41,45,50,50	0
3	EDO	N	406	4/4	0.72	0.29	5.50	57,58,64,65	0
3	EDO	L	403	4/4	0.83	0.33	5.47	59,59,63,63	0
4	PUT	E	401	6/6	0.95	0.32	5.43	36,37,43,45	0
5	PEG	K	406	7/7	0.90	0.28	5.19	52,81,94,96	0
3	EDO	K	405	4/4	0.88	0.24	5.03	51,59,62,63	0
2	GOL	C	403	6/6	0.94	0.22	4.99	43,57,66,67	0
5	PEG	D	406	7/7	0.84	0.26	4.85	57,72,84,89	0
3	EDO	P	403	4/4	0.91	0.32	4.69	75,77,79,80	0
3	EDO	F	403	4/4	0.89	0.25	4.31	54,63,64,73	0
4	PUT	C	401	6/6	0.97	0.30	4.10	36,38,41,44	0
2	GOL	N	404	6/6	0.94	0.20	4.08	44,51,60,61	0
2	GOL	E	405	6/6	0.81	0.35	4.08	71,83,91,92	0
4	PUT	D	402	6/6	0.97	0.27	3.99	37,41,44,45	0
2	GOL	J	404	6/6	0.85	0.24	3.84	61,73,77,80	0
3	EDO	M	403	4/4	0.78	0.21	3.64	62,65,71,71	0
4	PUT	J	401	6/6	0.96	0.33	3.62	38,40,42,43	0
2	GOL	F	402	6/6	0.89	0.24	3.43	57,66,70,71	0
4	PUT	B	401	6/6	0.95	0.28	3.40	39,40,40,40	0
3	EDO	D	404	4/4	0.83	0.27	3.26	62,65,75,75	0
4	PUT	K	401	6/6	0.94	0.28	3.20	41,42,45,45	0
2	GOL	P	401	6/6	0.84	0.26	2.72	75,79,82,83	0
2	GOL	M	402	6/6	0.96	0.16	2.71	44,54,70,70	0
2	GOL	L	402	6/6	0.91	0.13	2.42	45,55,58,59	0
2	GOL	A	402	6/6	0.82	0.23	2.04	59,66,75,98	0
3	EDO	C	404	4/4	0.88	0.21	2.02	52,57,63,63	0
2	GOL	K	402	6/6	0.95	0.17	1.98	48,59,59,69	0
2	GOL	D	401	6/6	0.95	0.15	1.79	49,57,75,78	0
2	GOL	G	403	6/6	0.94	0.18	1.63	46,60,62,65	0
2	GOL	K	403	6/6	0.95	0.13	1.59	45,52,63,67	0
2	GOL	E	402	6/6	0.91	0.15	1.53	51,64,78,84	0
2	GOL	E	403	6/6	0.95	0.17	1.40	62,71,87,99	0
3	EDO	I	403	4/4	0.87	0.19	1.32	55,82,83,85	0
2	GOL	C	402	6/6	0.96	0.14	1.21	45,52,69,77	0
3	EDO	I	402	4/4	0.94	0.19	1.16	53,58,60,69	0
2	GOL	O	402	6/6	0.91	0.15	1.09	59,64,68,73	0
2	GOL	B	403	6/6	0.91	0.14	1.05	53,67,70,73	0
3	EDO	A	403	4/4	0.95	0.16	0.87	52,61,61,65	0
2	GOL	N	403	6/6	0.91	0.15	0.77	44,58,71,75	0
2	GOL	B	402	6/6	0.93	0.11	0.48	49,55,62,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	GOL	G	402	6/6	0.86	0.16	0.46	79,88,91,94	0
2	GOL	N	401	6/6	0.97	0.11	0.08	46,58,69,73	0
2	GOL	J	402	6/6	0.96	0.10	0.07	45,52,58,66	0
3	EDO	P	402	4/4	0.81	0.22	-0.33	69,80,85,86	0
3	EDO	F	404	4/4	0.90	0.43	-	71,72,75,79	0
3	EDO	B	404	4/4	0.65	0.20	-	71,72,89,91	0
3	EDO	L	404	4/4	0.84	0.20	-	70,78,84,85	0
3	EDO	D	405	4/4	0.85	0.19	-	69,75,75,80	0
3	EDO	B	405	4/4	0.88	0.21	-	49,62,74,83	0

6.5 Other polymers

There are no such residues in this entry.