Full wwPDB X-ray Structure Validation Report (i)

Sep 19, 2023 – 12:05 PM 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

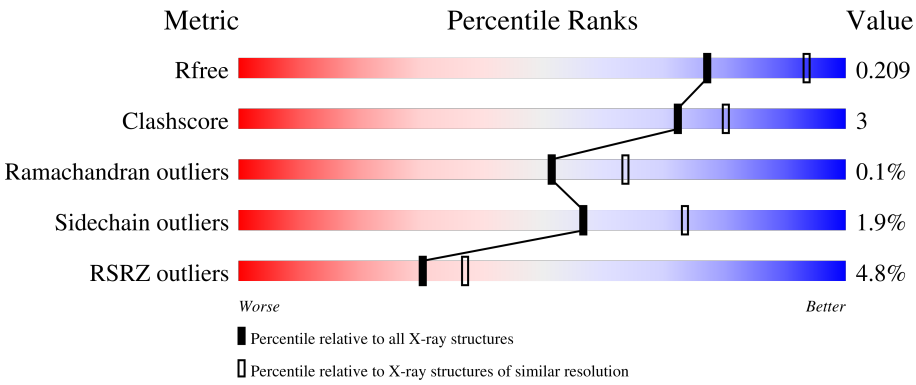
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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%

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Mol	Chain	Length	Quality of chain
1	F	304	%, 89%, 8%
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	L	402	-	-	X	-

2 Entry composition (i)

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

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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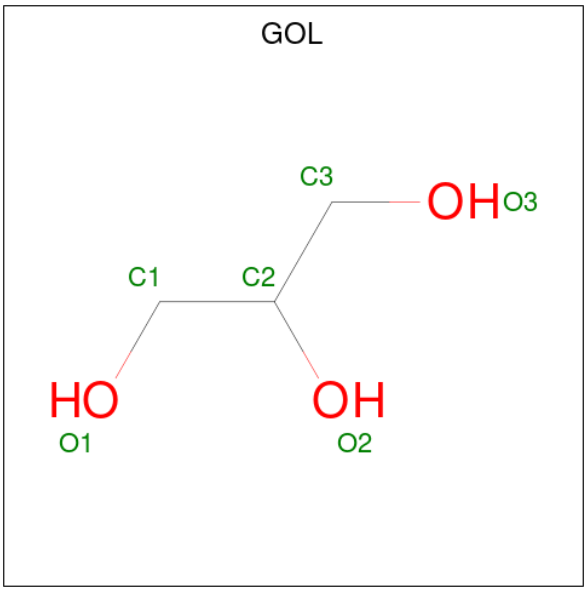
Chain	Residue	Modelled	Actual	Comment	Reference
K	0	ALA	-	expression tag	UNP G7ITU5
K	158	SER	CYS	engineered mutation	UNP G7ITU5
L	-2	SER	-	expression tag	UNP G7ITU5
L	-1	ASN	-	expression tag	UNP G7ITU5
L	0	ALA	-	expression tag	UNP G7ITU5
L	158	SER	CYS	engineered mutation	UNP G7ITU5
M	-2	SER	-	expression 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
			Total	C	O		
2	A	1	6	3	3	0	0
2	A	1	6	3	3	0	0
2	B	1	6	3	3	0	0
2	B	1	6	3	3	0	0
2	C	1	6	3	3	0	0
2	C	1	6	3	3	0	0
2	D	1	6	3	3	0	0
2	D	1	6	3	3	0	0
2	E	1	6	3	3	0	0
2	E	1	6	3	3	0	0
2	E	1	6	3	3	0	0
2	E	1	6	3	3	0	0
2	F	1	6	3	3	0	0
2	G	1	6	3	3	0	0
2	G	1	6	3	3	0	0
2	I	1	6	3	3	0	0
2	J	1	6	3	3	0	0
2	J	1	6	3	3	0	0
2	J	1	6	3	3	0	0
2	K	1	6	3	3	0	0
2	K	1	6	3	3	0	0
2	K	1	6	3	3	0	0

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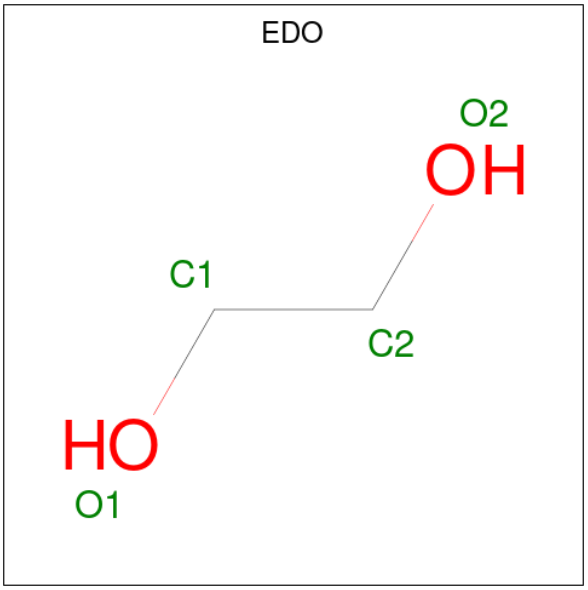
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	L	1	6	3	3	0	0
2	M	1	6	3	3	0	0
2	N	1	6	3	3	0	0
2	N	1	6	3	3	0	0
2	N	1	6	3	3	0	0
2	N	1	6	3	3	0	0
2	O	1	6	3	3	0	0
2	P	1	6	3	3	0	0

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



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

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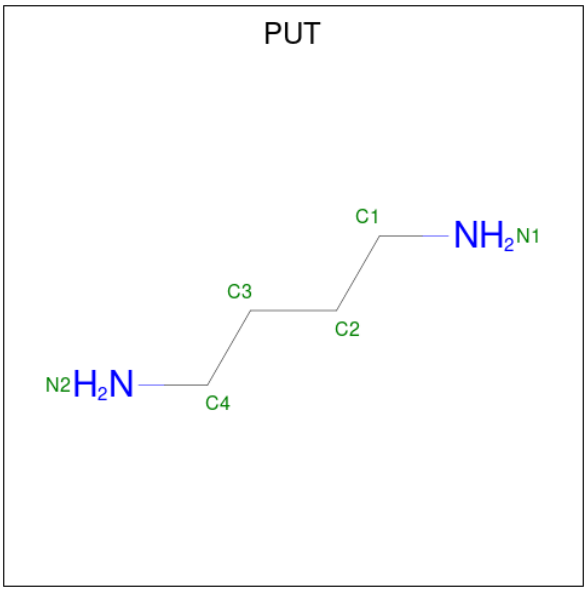
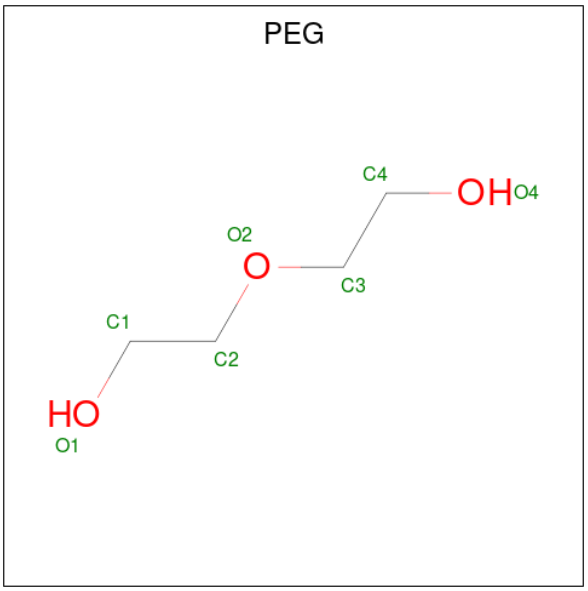
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
3	C	1	4	2	2		0	0
3	D	1	4	2	2		0	0
3	D	1	4	2	2		0	0
3	F	1	4	2	2		0	0
3	F	1	4	2	2		0	0
3	I	1	4	2	2		0	0
3	I	1	4	2	2		0	0
3	K	1	4	2	2		0	0
3	L	1	4	2	2		0	0
3	L	1	4	2	2		0	0
3	M	1	4	2	2		0	0
3	N	1	4	2	2		0	0
3	P	1	4	2	2		0	0
3	P	1	4	2	2		0	0

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
4	B	1	6	4	2	0	0
4	C	1	6	4	2	0	0
4	D	1	6	4	2	0	0
4	E	1	6	4	2	0	0
4	F	1	6	4	2	0	0
4	G	1	6	4	2	0	0
4	J	1	6	4	2	0	0
4	K	1	6	4	2	0	0
4	L	1	6	4	2	0	0
4	M	1	6	4	2	0	0
4	N	1	6	4	2	0	0
4	O	1	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
			Total	C	O		
5	D	1	7	4	3	0	0
			Total	C	O		
5	K	1	7	4	3	0	0
			Total	C	O		
5	L	1	7	4	3	0	0

- Molecule 6 is water.

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

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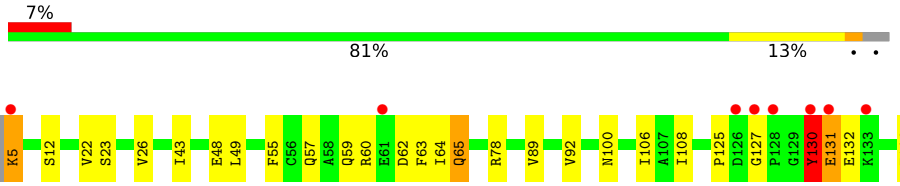
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	J	257	257	257	0	0
			Total	O		
6	K	270	270	270	0	0
			Total	O		
6	L	292	292	292	0	0
			Total	O		
6	M	279	279	279	0	0
			Total	O		
6	N	291	291	291	0	0
			Total	O		
6	O	226	226	226	0	0
			Total	O		
6	P	106	106	106	0	0

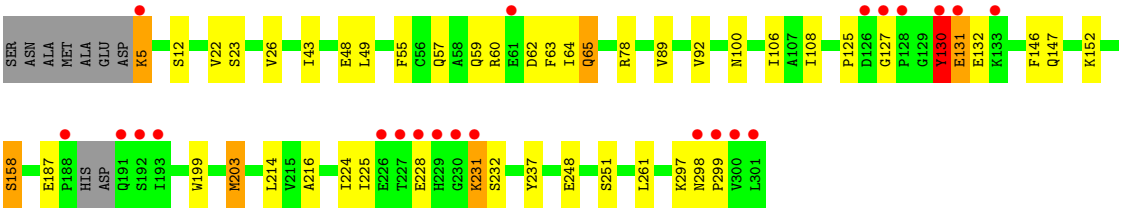
3 Residue-property plots (i)

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

• Molecule 1: N-carbamoylputrescine amidohydrolase

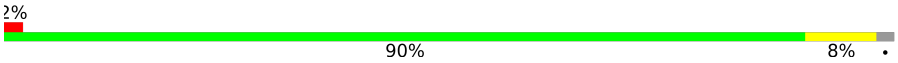
Chain A:

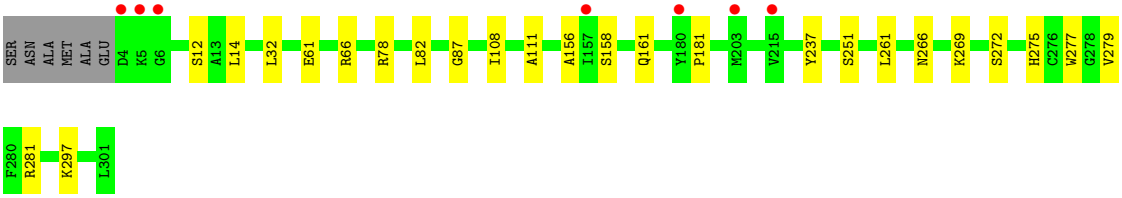




• Molecule 1: N-carbamoylputrescine amidohydrolase

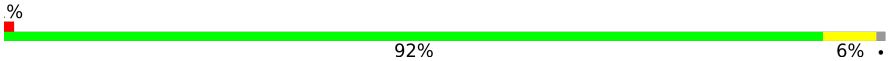
Chain B:





• Molecule 1: N-carbamoylputrescine amidohydrolase

Chain C:

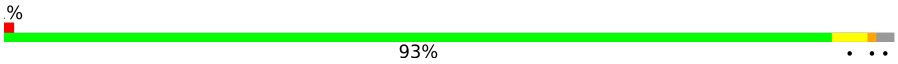


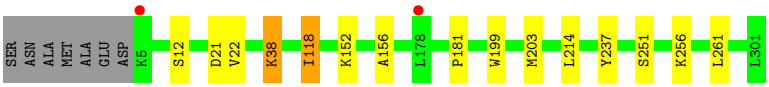
• Molecule 1: N-carbamoylputrescine amidohydrolase

Chain D:

• Molecule 1: N-carbamoylputrescine amidohydrolase

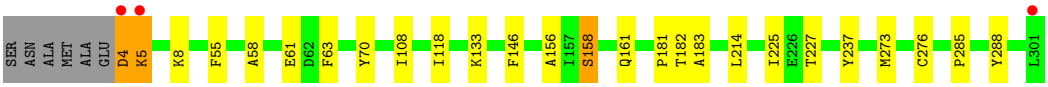
Chain E:





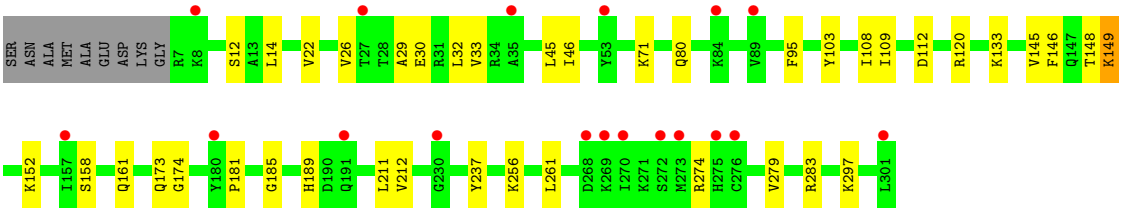
• Molecule 1: N-carbamoylputrescine amidohydrolase

Chain F:



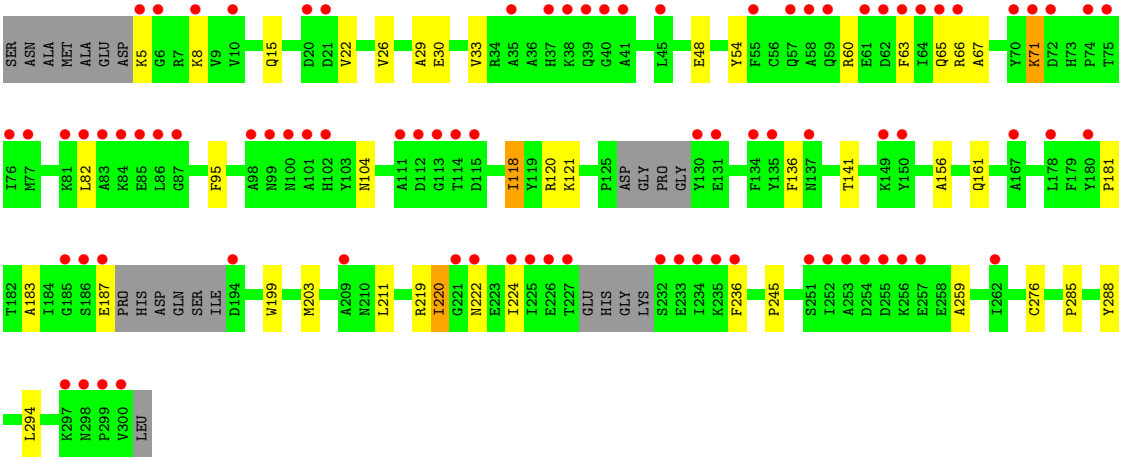
• Molecule 1: N-carbamoylputrescine amidohydrolase

Chain G:



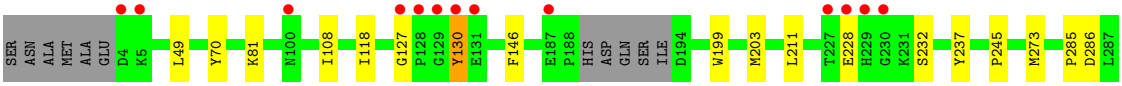
• Molecule 1: N-carbamoylputrescine amidohydrolase

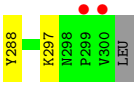
Chain H:



• Molecule 1: N-carbamoylputrescine amidohydrolase

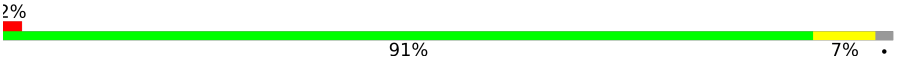
Chain I:

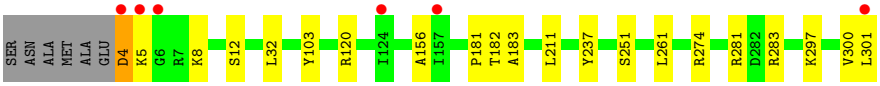




• Molecule 1: N-carbamoylputrescine amidohydrolase

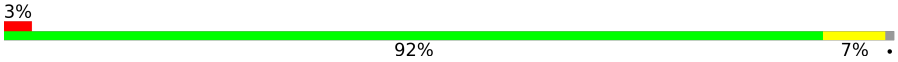
Chain J:

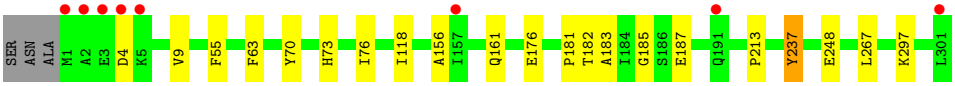




• Molecule 1: N-carbamoylputrescine amidohydrolase

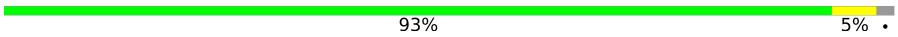
Chain K:





• Molecule 1: N-carbamoylputrescine amidohydrolase

Chain L:

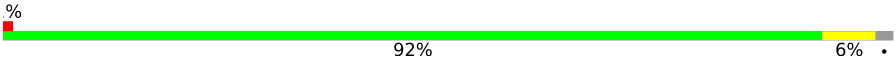


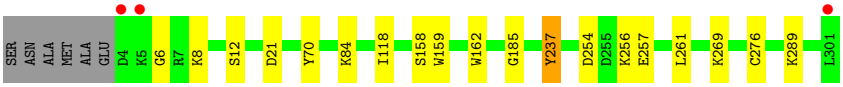
• Molecule 1: N-carbamoylputrescine amidohydrolase

Chain M:

• Molecule 1: N-carbamoylputrescine amidohydrolase

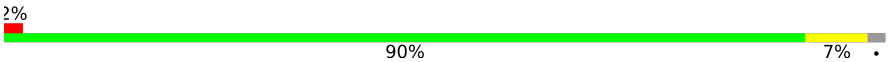
Chain N:

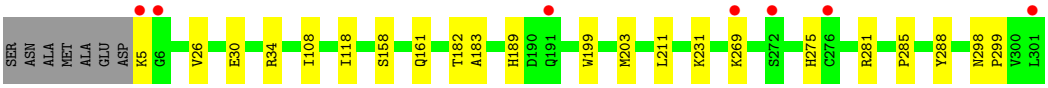




• Molecule 1: N-carbamoylputrescine amidohydrolase

Chain O:

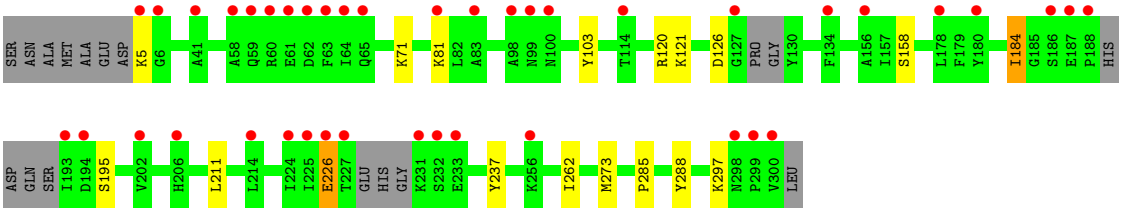




• Molecule 1: N-carbamoylputrescine amidohydrolase

Chain P:

13%
88%
5% • 6%


SER ASN ALA MET ALA GLU ASP K5 G6 A41 A58 Q59 R60 E61 D62 F63 I64 Q65 K71 K81 L82 A83 A98 N99 N100 Y103 T114 R120 K121 D126 G127 PRO GLY Y130 F134 A156 I157 S158 L178 F179 Y180 I184 G185 S186 E187 P188 HIS
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 N298 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 (1.00%)	wwPDB-VP
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 , 37.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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
1:A:55:PHE:HB2	1:A:63:PHE:CD2	2.32	0.64
3:A:403:EDO:H21	6:C:615:HOH:O	1.98	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:N	1:A:5:LYS:CD	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:HE3	1:H:71:LYS:HA	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:5:LYS:CD	6:A:660:HOH:O	2.52	0.52
1:A:127:GLY:CA	6:A:549:HOH:O	2.56	0.52
1:M:191:GLN:O	1:M:191:GLN:HG2	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:22:VAL:HG23	6:G:574:HOH:O	2.10	0.50
1:G:185:GLY:HA2	1:G:237:TYR:CD2	2.46	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:CD2	1:O:189:HIS:H	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:C	1:E:214:LEU:HD23	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:C	1:L:214:LEU:HD23	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:CD	1:I:228:GLU:H	2.21	0.44
1:J:12:SER:HA	1:J:261:LEU:O	2.18	0.44
1:K:9:VAL:HG21	1:K:267:LEU:CD1	2.48	0.44
1:K:185:GLY:HA2	1:K:237:TYR:CD2	2.53	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:61:GLU:HG3	1:H:276[A]:CYS:HB2	2.00	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: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:30:GLU:HG2	1:D:82:LEU:HD22	2.00	0.43
1:D:118:ILE:HD13	1:D:118:ILE:HG21	1.79	0.43
1:G:80:GLN:HG2	1:G:109:ILE:HD12	2.01	0.43
1:G:211:LEU:HD23	1:G:274:ARG:N	2.33	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:OD1	1:I:286:ASP:N	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:CD	1:A:228:GLU:H	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:4:ASP:OD1	1:D:269:LYS:NZ	2.51	0.42
1:D:297:LYS:HE2	1:D:297:LYS:HB3	1.78	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:HD12	1:B:108:ILE:N	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
6:A:564:HOH:O	3:B:405:EDO:H11	2.19	0.42
1:B:14:LEU:HD22	1:B:32:LEU:HB3	2.02	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:HD23	1:L:79:LEU:HA	1.83	0.42
1:F:55:PHE:HB2	1:F:63:PHE:CD2	2.54	0.42
1:F:156:ALA:O	1:F:181:PRO:HD2	2.20	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:HD23	1:I:49:LEU:HA	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:15:GLN:HB3	1:H:259:ALA:HB3	2.01	0.41
1:H:118:ILE:HD12	1:H:118:ILE:H	1.85	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:HD13	1:E:118:ILE:HG21	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:22:VAL:O	1:A:26:VAL:HG23	2.21	0.41
1:A:187:GLU:HG2	6:A:670:HOH:O	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:HD12	1:B:82:LEU:HA	1.88	0.40
1:G:22:VAL:O	1:G:26:VAL:HG23	2.21	0.40
1:H:65:GLN:OE1	1:H:65:GLN:HA	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%)	41	50
1	B	297/304 (98%)	285 (96%)	11 (4%)	1 (0%)	41	50
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%)	41	50
1	G	293/304 (96%)	281 (96%)	11 (4%)	1 (0%)	41	50
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%)	41	50
1	N	296/304 (97%)	286 (97%)	9 (3%)	1 (0%)	41	50
1	O	296/304 (97%)	285 (96%)	10 (3%)	1 (0%)	41	50
1	P	280/304 (92%)	271 (97%)	9 (3%)	0	100	100
All	All	4701/4864 (97%)	4520 (96%)	174 (4%)	7 (0%)	51	64

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%)	22	31
1	B	249/252 (99%)	244 (98%)	5 (2%)	55	72
1	C	251/252 (100%)	247 (98%)	4 (2%)	62	78
1	D	250/252 (99%)	249 (100%)	1 (0%)	91	96
1	E	247/252 (98%)	244 (99%)	3 (1%)	71	84
1	F	249/252 (99%)	243 (98%)	6 (2%)	49	66
1	G	246/252 (98%)	239 (97%)	7 (3%)	43	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	236/252 (94%)	227 (96%)	9 (4%)	33	47
1	I	243/252 (96%)	239 (98%)	4 (2%)	62	78
1	J	249/252 (99%)	243 (98%)	6 (2%)	49	66
1	K	251/252 (100%)	248 (99%)	3 (1%)	71	84
1	L	250/252 (99%)	249 (100%)	1 (0%)	91	96
1	M	249/252 (99%)	246 (99%)	3 (1%)	71	84
1	N	248/252 (98%)	246 (99%)	2 (1%)	81	91
1	O	248/252 (98%)	246 (99%)	2 (1%)	81	91
1	P	240/252 (95%)	232 (97%)	8 (3%)	38	53
All	All	3953/4032 (98%)	3876 (98%)	77 (2%)	57	73

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

Sometimes 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 (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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	F	402	-	5,5,5	0.51	0	5,5,5	0.24	0
2	GOL	M	402	-	5,5,5	0.40	0	5,5,5	0.21	0
3	EDO	L	403	-	3,3,3	0.54	0	2,2,2	0.24	0
5	PEG	D	406	-	6,6,6	0.68	0	5,5,5	0.19	0
2	GOL	N	405	-	5,5,5	0.65	0	5,5,5	0.52	0
3	EDO	B	404	-	3,3,3	0.61	0	2,2,2	0.15	0
2	GOL	D	401	-	5,5,5	0.42	0	5,5,5	0.31	0
2	GOL	K	404	-	5,5,5	0.53	0	5,5,5	0.27	0
3	EDO	C	404	-	3,3,3	0.71	0	2,2,2	0.42	0
2	GOL	I	401	-	5,5,5	0.47	0	5,5,5	0.17	0
2	GOL	E	404	-	5,5,5	0.36	0	5,5,5	0.32	0
3	EDO	A	403	-	3,3,3	0.51	0	2,2,2	0.31	0
2	GOL	K	402	-	5,5,5	0.61	0	5,5,5	0.41	0
2	GOL	O	402	-	5,5,5	0.25	0	5,5,5	0.67	0
2	GOL	J	403	-	5,5,5	0.57	0	5,5,5	0.70	0
4	PUT	M	401	-	5,5,5	0.47	0	4,4,4	0.66	0
4	PUT	K	401	-	5,5,5	0.38	0	4,4,4	0.63	0
4	PUT	O	401	-	5,5,5	0.35	0	4,4,4	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	PUT	B	401	-	5,5,5	0.34	0	4,4,4	0.76	0
2	GOL	D	403	-	5,5,5	0.79	0	5,5,5	0.51	0
2	GOL	A	402	-	5,5,5	0.47	0	5,5,5	0.23	0
3	EDO	N	406	-	3,3,3	0.61	0	2,2,2	0.02	0
2	GOL	N	403	-	5,5,5	0.78	0	5,5,5	0.64	0
2	GOL	E	402	-	5,5,5	0.37	0	5,5,5	0.36	0
2	GOL	P	401	-	5,5,5	0.44	0	5,5,5	0.15	0
3	EDO	L	404	-	3,3,3	0.55	0	2,2,2	0.12	0
2	GOL	G	403	-	5,5,5	0.46	0	5,5,5	0.24	0
3	EDO	P	402	-	3,3,3	0.60	0	2,2,2	0.21	0
5	PEG	K	406	-	6,6,6	0.59	0	5,5,5	0.14	0
2	GOL	J	404	-	5,5,5	0.34	0	5,5,5	0.30	0
4	PUT	F	401	-	5,5,5	0.36	0	4,4,4	0.46	0
2	GOL	N	404	-	5,5,5	0.46	0	5,5,5	0.24	0
2	GOL	J	402	-	5,5,5	0.38	0	5,5,5	0.39	0
3	EDO	I	403	-	3,3,3	0.51	0	2,2,2	0.43	0
3	EDO	P	403	-	3,3,3	0.53	0	2,2,2	0.29	0
2	GOL	B	402	-	5,5,5	0.69	0	5,5,5	0.59	0
3	EDO	D	405	-	3,3,3	0.50	0	2,2,2	0.35	0
4	PUT	L	401	-	5,5,5	0.43	0	4,4,4	0.77	0
4	PUT	N	402	-	5,5,5	0.28	0	4,4,4	0.61	0
2	GOL	A	401	-	5,5,5	0.59	0	5,5,5	0.64	0
4	PUT	C	401	-	5,5,5	0.26	0	4,4,4	0.92	0
4	PUT	E	401	-	5,5,5	0.18	0	4,4,4	0.84	0
4	PUT	J	401	-	5,5,5	0.40	0	4,4,4	0.98	0
2	GOL	C	402	-	5,5,5	0.43	0	5,5,5	0.47	0
5	PEG	L	405	-	6,6,6	0.59	0	5,5,5	0.34	0
2	GOL	E	405	-	5,5,5	0.58	0	5,5,5	0.43	0
3	EDO	D	404	-	3,3,3	0.63	0	2,2,2	0.24	0
3	EDO	F	403	-	3,3,3	0.61	0	2,2,2	0.21	0
3	EDO	I	402	-	3,3,3	0.65	0	2,2,2	0.05	0
4	PUT	G	401	-	5,5,5	0.22	0	4,4,4	1.11	1 (25%)
3	EDO	M	403	-	3,3,3	0.78	0	2,2,2	0.13	0
2	GOL	B	403	-	5,5,5	0.31	0	5,5,5	0.36	0
2	GOL	L	402	-	5,5,5	0.79	0	5,5,5	0.51	0
3	EDO	F	404	-	3,3,3	0.59	0	2,2,2	0.30	0
2	GOL	G	402	-	5,5,5	0.44	0	5,5,5	0.58	0
2	GOL	C	403	-	5,5,5	0.51	0	5,5,5	0.41	0
3	EDO	K	405	-	3,3,3	0.60	0	2,2,2	0.11	0
3	EDO	B	405	-	3,3,3	0.69	0	2,2,2	0.02	0
4	PUT	D	402	-	5,5,5	0.21	0	4,4,4	0.82	0
2	GOL	E	403	-	5,5,5	0.48	0	5,5,5	0.44	0
2	GOL	K	403	-	5,5,5	0.65	0	5,5,5	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GOL	N	401	-	5,5,5	0.23	0	5,5,5	0.23	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	F	402	-	-	4/4/4/4	-
2	GOL	M	402	-	-	4/4/4/4	-
3	EDO	L	403	-	-	0/1/1/1	-
5	PEG	D	406	-	-	1/4/4/4	-
2	GOL	N	405	-	-	4/4/4/4	-
3	EDO	B	404	-	-	1/1/1/1	-
2	GOL	D	401	-	-	2/4/4/4	-
2	GOL	K	404	-	-	4/4/4/4	-
3	EDO	C	404	-	-	0/1/1/1	-
2	GOL	I	401	-	-	2/4/4/4	-
2	GOL	E	404	-	-	2/4/4/4	-
3	EDO	A	403	-	-	1/1/1/1	-
2	GOL	K	402	-	-	4/4/4/4	-
2	GOL	O	402	-	-	3/4/4/4	-
2	GOL	J	403	-	-	2/4/4/4	-
4	PUT	M	401	-	-	0/3/3/3	-
4	PUT	K	401	-	-	0/3/3/3	-
4	PUT	O	401	-	-	0/3/3/3	-
4	PUT	B	401	-	-	0/3/3/3	-
2	GOL	D	403	-	-	2/4/4/4	-
2	GOL	A	402	-	-	4/4/4/4	-
3	EDO	N	406	-	-	0/1/1/1	-
2	GOL	N	403	-	-	1/4/4/4	-
2	GOL	E	402	-	-	2/4/4/4	-
2	GOL	P	401	-	-	4/4/4/4	-
3	EDO	L	404	-	-	1/1/1/1	-
2	GOL	G	403	-	-	4/4/4/4	-
3	EDO	P	402	-	-	1/1/1/1	-
5	PEG	K	406	-	-	3/4/4/4	-
2	GOL	J	404	-	-	3/4/4/4	-
4	PUT	F	401	-	-	0/3/3/3	-

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	401	PUT	C2-C3-C4	-2.03	99.39	113.77

There are no chirality outliers.

All (100) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	402	GOL	O1-C1-C2-C3
2	B	402	GOL	O1-C1-C2-C3
2	C	403	GOL	O1-C1-C2-C3
2	D	401	GOL	C1-C2-C3-O3
2	D	401	GOL	O2-C2-C3-O3
2	E	403	GOL	C1-C2-C3-O3
2	F	402	GOL	C1-C2-C3-O3
2	G	403	GOL	O1-C1-C2-C3
2	I	401	GOL	O1-C1-C2-C3
2	J	404	GOL	C1-C2-C3-O3
2	J	404	GOL	O2-C2-C3-O3
2	K	402	GOL	O1-C1-C2-C3
2	K	402	GOL	C1-C2-C3-O3
2	K	403	GOL	O1-C1-C2-C3
2	K	403	GOL	O2-C2-C3-O3
2	K	404	GOL	O1-C1-C2-C3
2	L	402	GOL	O1-C1-C2-C3
2	M	402	GOL	C1-C2-C3-O3
2	N	405	GOL	O1-C1-C2-O2
2	N	405	GOL	C1-C2-C3-O3
2	B	402	GOL	O1-C1-C2-O2
2	K	404	GOL	O1-C1-C2-O2
2	N	401	GOL	O1-C1-C2-O2
5	L	405	PEG	O2-C3-C4-O4
2	A	401	GOL	O1-C1-C2-C3
2	A	402	GOL	C1-C2-C3-O3
2	B	402	GOL	C1-C2-C3-O3
2	C	402	GOL	O1-C1-C2-C3
2	C	403	GOL	C1-C2-C3-O3
2	D	403	GOL	C1-C2-C3-O3
2	E	402	GOL	O1-C1-C2-C3
2	E	404	GOL	C1-C2-C3-O3
2	E	405	GOL	O1-C1-C2-C3
2	F	402	GOL	O1-C1-C2-C3
2	G	402	GOL	C1-C2-C3-O3
2	G	403	GOL	C1-C2-C3-O3
2	J	402	GOL	O1-C1-C2-C3
2	J	402	GOL	C1-C2-C3-O3
2	J	403	GOL	C1-C2-C3-O3
2	K	403	GOL	C1-C2-C3-O3
2	K	404	GOL	C1-C2-C3-O3
2	L	402	GOL	C1-C2-C3-O3

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

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Mol	Chain	Res	Type	Atoms
3	I	402	EDO	O1-C1-C2-O2
2	C	403	GOL	O2-C2-C3-O3
2	E	402	GOL	O1-C1-C2-O2
2	K	403	GOL	O1-C1-C2-O2
5	L	405	PEG	O1-C1-C2-O2
2	D	403	GOL	O2-C2-C3-O3
5	D	406	PEG	O1-C1-C2-O2
3	F	404	EDO	O1-C1-C2-O2
2	N	404	GOL	C1-C2-C3-O3
5	K	406	PEG	C4-C3-O2-C2
2	L	402	GOL	O1-C1-C2-O2
2	A	402	GOL	O2-C2-C3-O3
2	P	401	GOL	O1-C1-C2-O2
2	P	401	GOL	O2-C2-C3-O3
3	L	404	EDO	O1-C1-C2-O2
2	J	404	GOL	O1-C1-C2-O2

There are no ring outliers.

16 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	403	EDO	2	0
2	D	401	GOL	1	0
3	C	404	EDO	2	0
3	A	403	EDO	2	0
2	K	402	GOL	1	0
4	K	401	PUT	1	0
2	D	403	GOL	1	0
2	A	401	GOL	2	0
3	D	404	EDO	1	0
3	F	403	EDO	1	0
3	I	402	EDO	1	0
2	B	403	GOL	1	0
2	L	402	GOL	4	0
2	C	403	GOL	1	0
3	K	405	EDO	1	0
3	B	405	EDO	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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	295/304 (97%)	-0.02	22 (7%)	14	19	28, 45, 95, 132	0
1	B	298/304 (98%)	-0.20	7 (2%)	60	67	25, 36, 59, 115	0
1	C	301/304 (99%)	-0.34	4 (1%)	77	81	25, 35, 54, 112	0
1	D	298/304 (98%)	-0.44	1 (0%)	94	96	24, 33, 49, 92	0
1	E	297/304 (97%)	-0.34	2 (0%)	87	91	26, 37, 57, 92	0
1	F	298/304 (98%)	-0.41	3 (1%)	82	86	28, 44, 64, 93	0
1	G	295/304 (97%)	0.44	18 (6%)	21	27	47, 65, 84, 101	0
1	H	282/304 (92%)	1.45	85 (30%)	0	0	50, 85, 118, 136	0
1	I	292/304 (96%)	-0.16	15 (5%)	28	35	28, 41, 84, 138	0
1	J	298/304 (98%)	-0.27	6 (2%)	65	71	26, 36, 58, 118	0
1	K	301/304 (99%)	-0.28	8 (2%)	54	62	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%)	-0.34	2 (0%)	87	91	25, 35, 52, 88	0
1	N	298/304 (98%)	-0.47	3 (1%)	82	86	25, 35, 52, 92	0
1	O	297/304 (97%)	-0.21	7 (2%)	59	66	32, 46, 66, 108	0
1	P	287/304 (94%)	0.69	41 (14%)	2	3	34, 61, 104, 119	0
All	All	4732/4864 (97%)	-0.09	225 (4%)	30	37	24, 40, 87, 138	0

All (225) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	58	ALA	7.4
1	H	300	VAL	7.3
1	J	4	ASP	6.9
1	B	4	ASP	6.3
1	A	230	GLY	6.3

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Mol	Chain	Res	Type	RSRZ
1	I	229	HIS	6.2
1	H	77	MET	6.0
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	H	227	THR	5.6
1	P	100	ASN	5.6
1	P	63	PHE	5.4
1	A	301	LEU	5.4
1	I	230	GLY	5.4
1	I	4	ASP	5.3
1	H	99	ASN	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	I	227	THR	4.6
1	B	5	LYS	4.6
1	P	232	SER	4.6
1	H	21	ASP	4.6
1	H	61	GLU	4.5
1	H	111	ALA	4.4
1	H	257	GLU	4.4
1	P	61	GLU	4.4
1	I	228	GLU	4.4
1	G	273	MET	4.3
1	H	100	ASN	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	P	5	LYS	4.2
1	H	298	ASN	4.2
1	A	192	SER	4.2
1	H	233	GLU	4.1
1	H	224	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
1	H	256	LYS	4.1
1	K	4	ASP	4.1
1	P	300	VAL	4.1
1	H	59	GLN	4.1
1	H	137	ASN	4.0
1	H	72	ASP	4.0
1	A	127	GLY	4.0
1	H	81	LYS	4.0
1	G	276	CYS	4.0
1	C	3	GLU	4.0
1	C	2	ALA	3.9
1	H	221	GLY	3.8
1	K	3	GLU	3.8
1	I	128	PRO	3.8
1	A	227	THR	3.8
1	H	85	GLU	3.7
1	H	102	HIS	3.7
1	H	65	GLN	3.7
1	J	5	LYS	3.7
1	H	74	PRO	3.7
1	H	299	PRO	3.7
1	H	178	LEU	3.7
1	P	65	GLN	3.7
1	O	6	GLY	3.6
1	P	188	PRO	3.6
1	P	298	ASN	3.6
1	D	4	ASP	3.6
1	F	5	LYS	3.6
1	H	226	GLU	3.6
1	H	112	ASP	3.6
1	P	225	ILE	3.6
1	P	256	LYS	3.6
1	P	134	PHE	3.6
1	H	6	GLY	3.6
1	A	299	PRO	3.6
1	H	253	ALA	3.5
1	P	99	ASN	3.5
1	P	226	GLU	3.5
1	H	180	TYR	3.5
1	H	187	GLU	3.5
1	P	231	LYS	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	194	ASP	3.4
1	H	87	GLY	3.4
1	H	254	ASP	3.3
1	L	4	ASP	3.3
1	H	40	GLY	3.3
1	A	126	ASP	3.3
1	P	98	ALA	3.3
1	A	226	GLU	3.3
1	H	8	LYS	3.3
1	H	222	ASN	3.3
1	J	6	GLY	3.3
1	A	188	PRO	3.3
1	H	114	THR	3.3
1	H	98	ALA	3.2
1	I	129	GLY	3.2
1	H	63	PHE	3.2
1	K	2	ALA	3.2
1	H	38	LYS	3.2
1	A	191	GLN	3.2
1	H	57	GLN	3.2
1	H	83	ALA	3.2
1	H	66	ARG	3.2
1	P	62	ASP	3.1
1	G	272	SER	3.1
1	H	131	GLU	3.0
1	P	178	LEU	3.0
1	A	133	LYS	3.0
1	H	135	TYR	3.0
1	H	255	ASP	3.0
1	P	299	PRO	3.0
1	G	35	ALA	3.0
1	E	5	LYS	3.0
1	H	130	TYR	2.9
1	C	4	ASP	2.9
1	F	301	LEU	2.9
1	O	276[A]	CYS	2.9
1	P	127	GLY	2.9
1	H	236	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	I	299	PRO	2.9
1	P	224	ILE	2.9
1	H	82	LEU	2.9
1	H	20	ASP	2.9
1	N	4	ASP	2.8
1	P	156	ALA	2.8
1	H	167	ALA	2.8
1	G	268	ASP	2.8
1	P	59	GLN	2.8
1	C	1	MET	2.8
1	H	150	TYR	2.8
1	H	41	ALA	2.8
1	P	186	SER	2.8
1	H	113	GLY	2.7
1	B	6	GLY	2.7
1	A	300	VAL	2.7
1	A	61	GLU	2.7
1	I	100	ASN	2.7
1	H	84	LYS	2.7
1	H	297	LYS	2.7
1	H	235	LYS	2.6
1	H	35	ALA	2.6
1	H	101	ALA	2.6
1	H	71	LYS	2.6
1	N	301	LEU	2.6
1	H	209	ALA	2.6
1	H	76	ILE	2.6
1	G	301	LEU	2.6
1	P	6	GLY	2.6
1	H	149	LYS	2.6
1	P	233	GLU	2.5
1	G	84	LYS	2.5
1	B	157	ILE	2.5
1	G	270	ILE	2.5
1	P	180	TYR	2.5
1	P	214	LEU	2.5
1	H	115	ASP	2.5
1	P	194	ASP	2.5
1	G	89	VAL	2.4
1	H	39	GLN	2.4
1	G	27	THR	2.4
1	H	64	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	45	LEU	2.4
1	H	37	HIS	2.4
1	M	5	LYS	2.4
1	G	157	ILE	2.4
1	P	114	THR	2.4
1	I	131	GLU	2.4
1	P	202	VAL	2.4
1	H	5	LYS	2.3
1	O	191	GLN	2.3
1	P	60	ARG	2.3
1	I	127	GLY	2.3
1	J	157	ILE	2.3
1	A	231	LYS	2.3
1	G	8	LYS	2.3
1	H	251	SER	2.3
1	J	301	LEU	2.3
1	O	272	SER	2.3
1	G	53	TYR	2.3
1	K	5	LYS	2.3
1	B	215	VAL	2.2
1	H	262	ILE	2.2
1	O	269	LYS	2.2
1	I	300	VAL	2.2
1	A	298	ASN	2.2
1	M	178	LEU	2.2
1	K	191	GLN	2.2
1	N	5	LYS	2.2
1	J	124	ILE	2.2
1	G	269	LYS	2.2
1	H	70	TYR	2.2
1	A	131	GLU	2.2
1	P	41	ALA	2.2
1	A	5	LYS	2.2
1	G	275	HIS	2.2
1	H	252	ILE	2.2
1	I	187	GLU	2.1
1	E	178	LEU	2.1
1	I	5	LYS	2.1
1	G	230	GLY	2.1
1	B	203	MET	2.1
1	G	180	TYR	2.1
1	P	81	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	K	157	ILE	2.1
1	P	64	ILE	2.1
1	P	83	ALA	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	K	301	LEU	2.0
1	B	180	TYR	2.0
1	G	191	GLN	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 monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	B	404	4/4	0.65	0.20	71,72,89,91	0
3	EDO	N	406	4/4	0.72	0.29	57,58,64,65	0
3	EDO	M	403	4/4	0.78	0.21	62,65,71,71	0
2	GOL	N	405	6/6	0.78	0.29	62,69,85,89	0
2	GOL	E	405	6/6	0.81	0.35	71,83,91,92	0
3	EDO	P	402	4/4	0.81	0.22	69,80,85,86	0
2	GOL	A	402	6/6	0.82	0.23	59,66,75,98	0
2	GOL	A	401	6/6	0.83	0.19	55,74,75,75	0
3	EDO	D	404	4/4	0.83	0.27	62,65,75,75	0
3	EDO	L	403	4/4	0.83	0.33	59,59,63,63	0
5	PEG	L	405	7/7	0.83	0.37	62,68,83,83	0
2	GOL	J	403	6/6	0.84	0.23	62,64,74,80	0
3	EDO	L	404	4/4	0.84	0.20	70,78,84,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	PEG	D	406	7/7	0.84	0.26	57,72,84,89	0
2	GOL	P	401	6/6	0.84	0.26	75,79,82,83	0
3	EDO	D	405	4/4	0.85	0.19	69,75,75,80	0
2	GOL	J	404	6/6	0.85	0.24	61,73,77,80	0
2	GOL	G	402	6/6	0.86	0.16	79,88,91,94	0
3	EDO	I	403	4/4	0.87	0.19	55,82,83,85	0
2	GOL	D	403	6/6	0.87	0.39	48,60,69,72	0
3	EDO	B	405	4/4	0.88	0.21	49,62,74,83	0
3	EDO	K	405	4/4	0.88	0.24	51,59,62,63	0
3	EDO	C	404	4/4	0.88	0.20	52,57,63,63	0
4	PUT	G	401	6/6	0.89	0.39	66,68,72,76	0
3	EDO	F	403	4/4	0.89	0.24	54,63,64,73	0
2	GOL	F	402	6/6	0.89	0.24	57,66,70,71	0
5	PEG	K	406	7/7	0.90	0.28	52,81,94,96	0
3	EDO	F	404	4/4	0.90	0.42	71,72,75,79	0
2	GOL	O	402	6/6	0.91	0.15	59,64,68,73	0
3	EDO	P	403	4/4	0.91	0.32	75,77,79,80	0
2	GOL	B	403	6/6	0.91	0.14	53,67,70,73	0
2	GOL	L	402	6/6	0.91	0.13	45,55,58,59	0
2	GOL	N	403	6/6	0.91	0.15	44,58,71,75	0
2	GOL	E	402	6/6	0.91	0.15	51,64,78,84	0
2	GOL	I	401	6/6	0.92	0.14	54,60,69,70	0
2	GOL	K	404	6/6	0.92	0.28	53,58,64,71	0
2	GOL	B	402	6/6	0.93	0.11	49,55,62,67	0
2	GOL	E	404	6/6	0.94	0.22	49,54,60,61	0
4	PUT	F	401	6/6	0.94	0.32	59,62,67,67	0
2	GOL	C	403	6/6	0.94	0.22	43,57,66,67	0
4	PUT	K	401	6/6	0.94	0.28	41,42,45,45	0
3	EDO	I	402	4/4	0.94	0.19	53,58,60,69	0
2	GOL	G	403	6/6	0.94	0.18	46,60,62,65	0
2	GOL	N	404	6/6	0.94	0.20	44,51,60,61	0
2	GOL	K	402	6/6	0.95	0.17	48,59,59,69	0
2	GOL	K	403	6/6	0.95	0.13	45,52,63,67	0
2	GOL	D	401	6/6	0.95	0.15	49,57,75,78	0
4	PUT	O	401	6/6	0.95	0.28	47,48,50,50	0
3	EDO	A	403	4/4	0.95	0.16	52,61,61,65	0
4	PUT	B	401	6/6	0.95	0.28	39,40,40,40	0
4	PUT	E	401	6/6	0.95	0.32	36,37,43,45	0
2	GOL	J	402	6/6	0.96	0.10	45,52,58,66	0
4	PUT	M	401	6/6	0.96	0.32	34,35,37,39	0
4	PUT	N	402	6/6	0.96	0.36	47,47,49,51	0
2	GOL	M	402	6/6	0.96	0.16	44,54,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GOL	C	402	6/6	0.96	0.14	45,52,69,77	0
2	GOL	E	403	6/6	0.96	0.17	62,71,87,99	0
4	PUT	J	401	6/6	0.96	0.33	38,40,42,43	0
4	PUT	C	401	6/6	0.97	0.30	36,38,41,44	0
4	PUT	L	401	6/6	0.97	0.32	41,45,50,50	0
4	PUT	D	402	6/6	0.97	0.27	37,41,44,45	0
2	GOL	N	401	6/6	0.97	0.11	46,58,69,73	0

6.5 Other polymers (i)

There are no such residues in this entry.