



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 06:41 PM UTC

PDB ID : 5H8L / pdb_00005h8l
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 ⓘ symbol.

The types of validation reports are described at

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

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

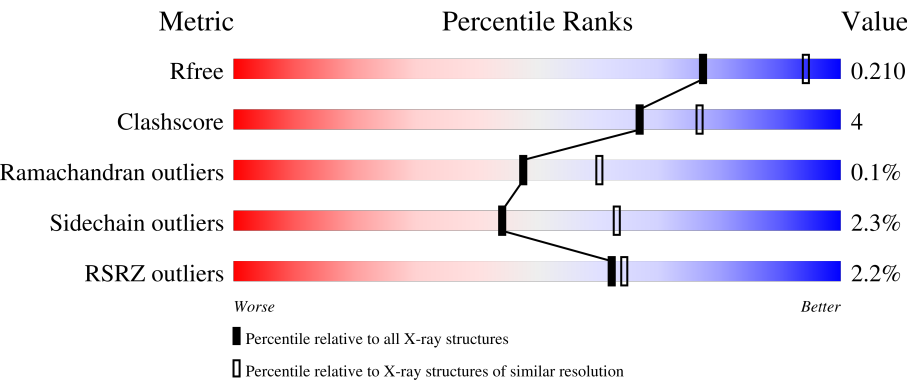
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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.



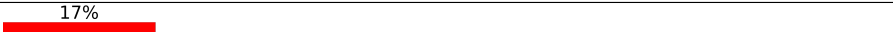
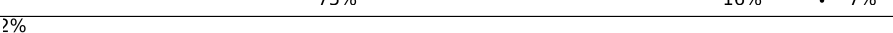
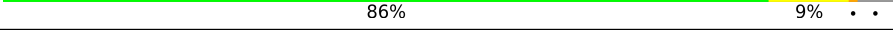
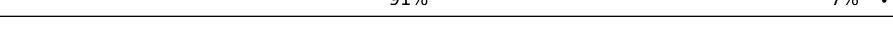
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	304	5% 79% 15%
1	B	304	88% 9%
1	C	304	% 90% 9%
1	D	304	89% 9%
1	E	304	91% 6%

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Mol	Chain	Length	Quality of chain
1	F	304	 89% 8% ..
1	G	304	 3% 82% 14% ..
1	H	304	 17% 75% 16% • 7%
1	I	304	 2% 86% 9% ..
1	J	304	 89% 8% ..
1	K	304	 % 91% 8% •
1	L	304	 91% 7% •
1	M	304	 88% 10% •
1	N	304	 88% 9% ..
1	O	304	 90% 6% ..
1	P	304	 4% 87% 6% • 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

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:

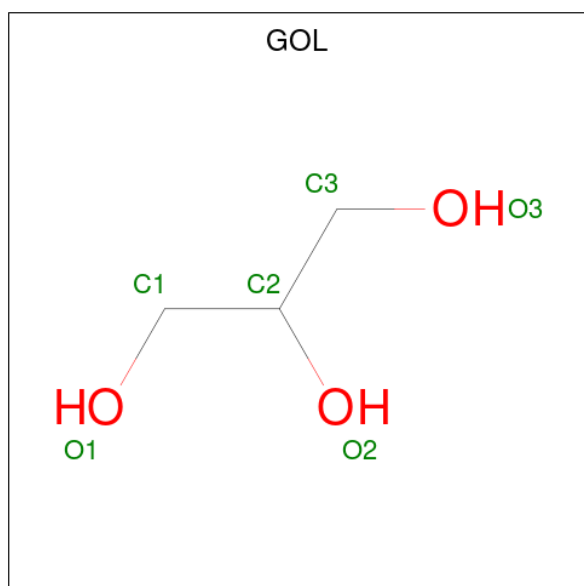
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP G7ITU5
A	-1	ASN	-	expression tag	UNP G7ITU5
A	0	ALA	-	expression tag	UNP G7ITU5
A	158	SER	CYS	engineered mutation	UNP G7ITU5
B	-2	SER	-	expression tag	UNP G7ITU5
B	-1	ASN	-	expression tag	UNP G7ITU5
B	0	ALA	-	expression tag	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 (CCD ID: GOL) (formula: $C_3H_8O_3$).



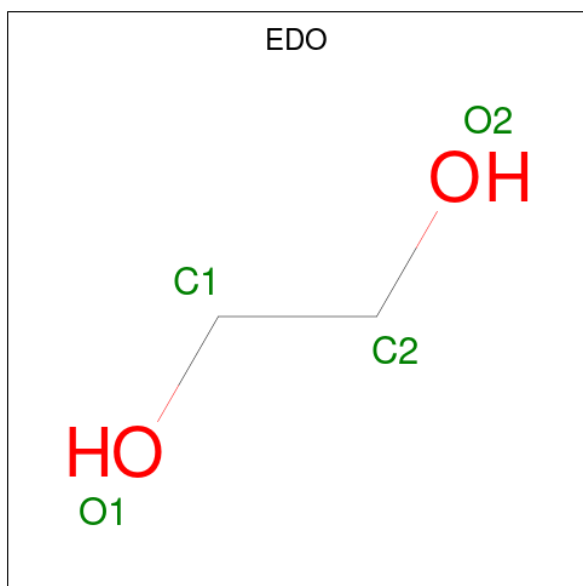
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total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

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

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



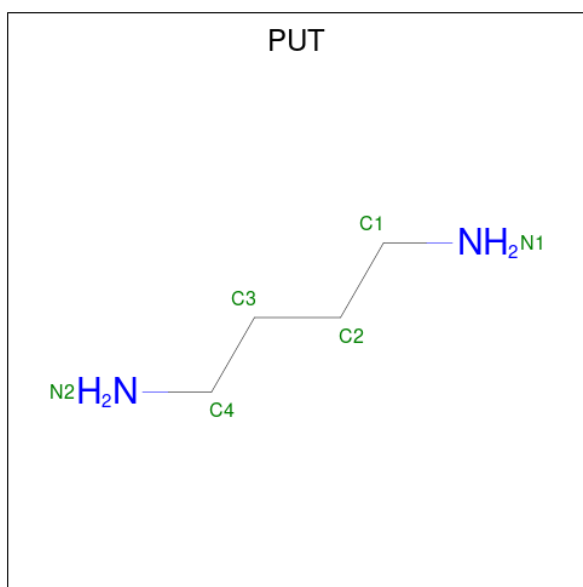
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

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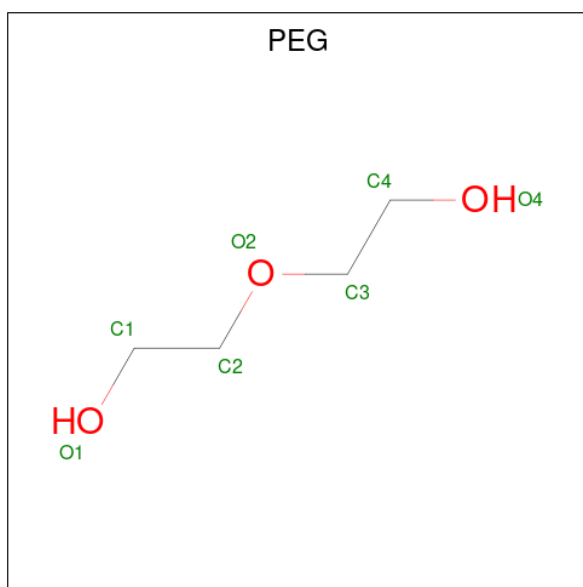
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	I	1	Total C O 4 2 2	0	0
3	I	1	Total C O 4 2 2	0	0
3	K	1	Total C O 4 2 2	0	0
3	L	1	Total C O 4 2 2	0	0
3	L	1	Total C O 4 2 2	0	0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

- Molecule 4 is 1,4-DIAMINOBUTANE (CCD ID: PUT) (formula: C₄H₁₂N₂).



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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 6 is water.

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

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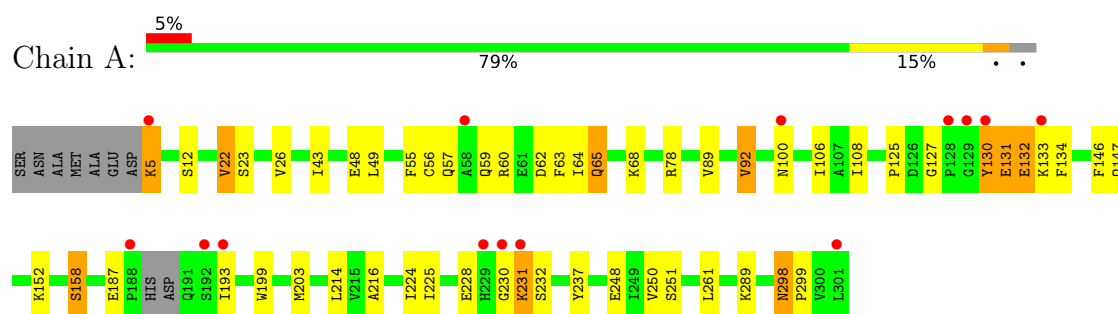
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	J	257	Total 257	O 257	0	0
6	K	270	Total 270	O 270	0	0
6	L	292	Total 292	O 292	0	0
6	M	279	Total 279	O 279	0	0
6	N	291	Total 291	O 291	0	0
6	O	226	Total 226	O 226	0	0
6	P	106	Total 106	O 106	0	0

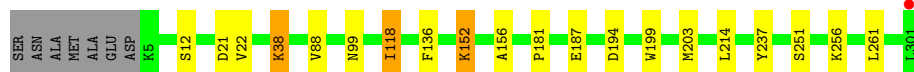
3 Residue-property plots [i](#)

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 E:  91% 6% ..



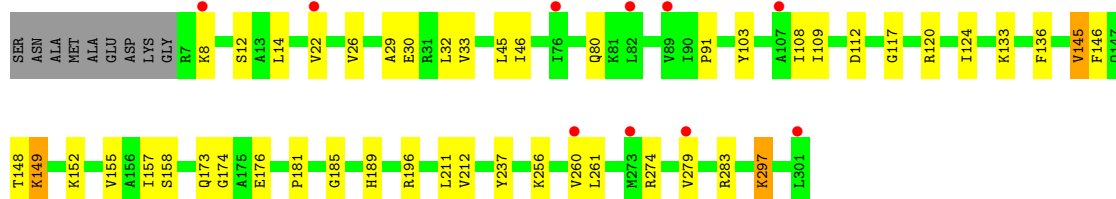
• Molecule 1: N-carbamoylputrescine amidohydrolase

Chain F:  89% 8% ..



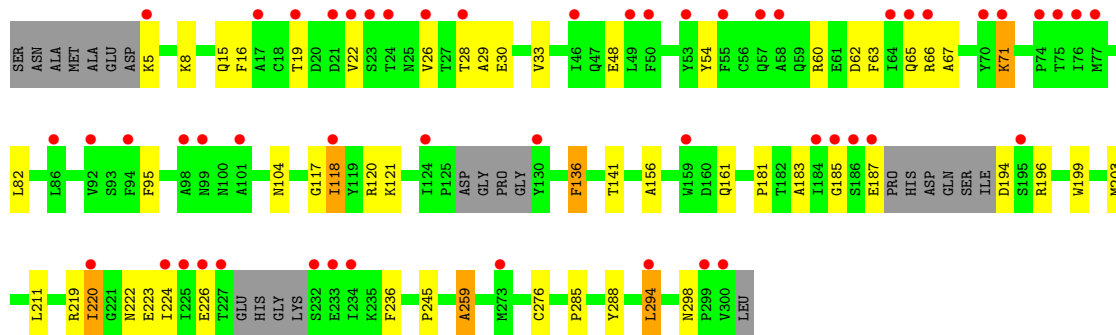
• Molecule 1: N-carbamoylputrescine amidohydrolase

Chain G:  3% 82% 14% ..



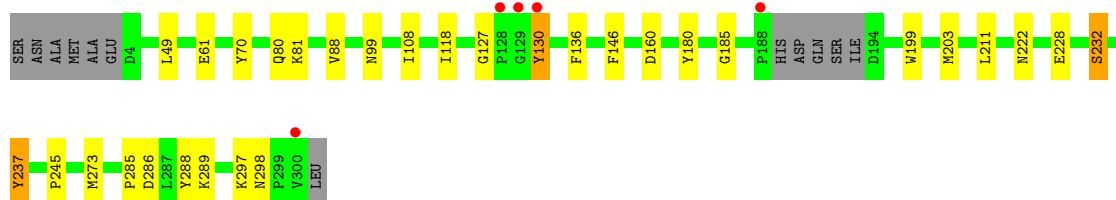
• Molecule 1: N-carbamoylputrescine amidohydrolase

Chain H:  17% 75% 16% 7%



• Molecule 1: N-carbamoylputrescine amidohydrolase

Chain I:  2% 86% 9% ..



• Molecule 1: N-carbamoylputrescine amidohydrolase

Chain J:  89% 8% ..



- Molecule 1: N-carbamoylputrescine amidohydrolase

Chain K:  91% 8% .



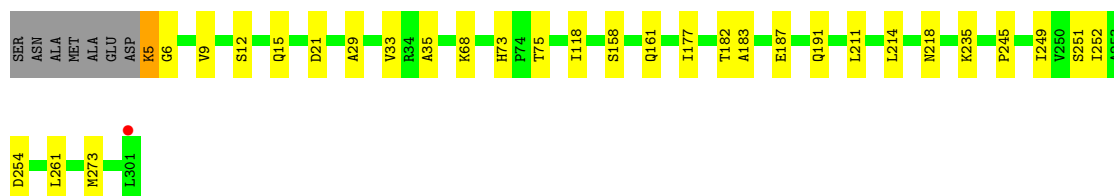
- Molecule 1: N-carbamoylputrescine amidohydrolase

Chain L:  91% 7% .



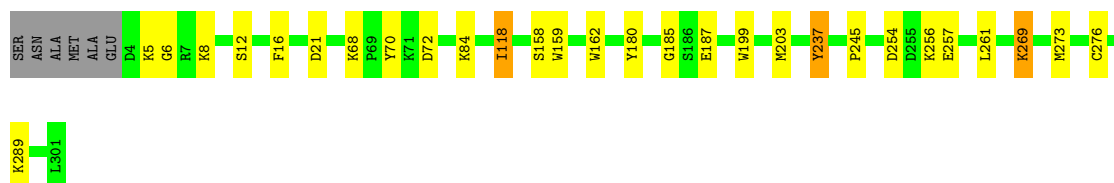
- Molecule 1: N-carbamoylputrescine amidohydrolase

Chain M:  88% 10% .



- Molecule 1: N-carbamoylputrescine amidohydrolase

Chain N:  88% 9% ..

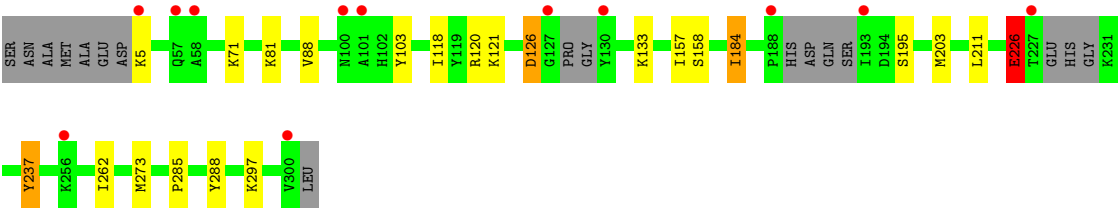
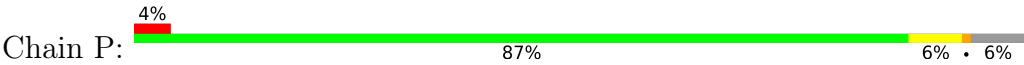


- Molecule 1: N-carbamoylputrescine amidohydrolase

Chain O:  90% 6% ..



- Molecule 1: N-carbamoylputrescine amidohydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	152.21Å 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) 98.0 (39.53-2.29)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.154 , 0.206 0.161 , 0.210	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)	0.34 , 52.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.15	2/2407 (0.1%)	1.10	11/3253 (0.3%)
1	B	1.17	1/2432 (0.0%)	1.08	2/3290 (0.1%)
1	C	1.19	4/2449 (0.2%)	1.09	4/3312 (0.1%)
1	D	1.16	2/2434 (0.1%)	1.06	3/3293 (0.1%)
1	E	1.10	1/2413 (0.0%)	1.05	4/3264 (0.1%)
1	F	1.10	0/2427	1.07	4/3283 (0.1%)
1	G	1.18	5/2400 (0.2%)	1.10	5/3248 (0.2%)
1	H	1.10	1/2300 (0.0%)	1.10	8/3107 (0.3%)
1	I	1.16	2/2375 (0.1%)	1.07	8/3212 (0.2%)
1	J	1.18	3/2427 (0.1%)	1.07	4/3283 (0.1%)
1	K	1.15	1/2449 (0.0%)	1.06	3/3312 (0.1%)
1	L	1.18	5/2434 (0.2%)	1.06	4/3293 (0.1%)
1	M	1.17	0/2426	1.05	3/3282 (0.1%)
1	N	1.21	3/2421 (0.1%)	1.09	8/3275 (0.2%)
1	O	1.06	0/2419	1.03	3/3272 (0.1%)
1	P	1.03	2/2337 (0.1%)	1.05	3/3157 (0.1%)
All	All	1.14	32/38550 (0.1%)	1.07	77/52136 (0.1%)

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	185	GLY	C-O	-7.05	1.16	1.23
1	P	126	ASP	CA-C	6.35	1.61	1.52
1	E	99	ASN	C-O	-6.34	1.18	1.24
1	C	38	LYS	C-O	-6.32	1.16	1.24
1	G	260	VAL	CA-C	6.24	1.59	1.52
1	H	226	GLU	N-CA	6.22	1.53	1.46
1	D	21	ASP	CA-C	6.17	1.60	1.52
1	C	134	PHE	C-O	-6.09	1.16	1.24
1	J	297	LYS	CA-C	6.02	1.60	1.52
1	B	145	VAL	C-O	-5.76	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	188	PRO	C-O	-5.74	1.16	1.24
1	L	99	ASN	C-O	-5.71	1.19	1.24
1	P	126	ASP	N-CA	5.64	1.53	1.46
1	J	272	SER	CA-C	5.57	1.60	1.52
1	L	250	VAL	C-O	-5.55	1.18	1.24
1	K	188	PRO	C-O	-5.53	1.17	1.24
1	L	185	GLY	C-O	5.44	1.28	1.24
1	N	180	TYR	CA-C	5.39	1.58	1.52
1	N	269	LYS	C-O	-5.36	1.17	1.24
1	G	155	VAL	CA-C	5.35	1.59	1.52
1	I	232	SER	CA-C	5.29	1.59	1.52
1	A	193	ILE	CA-CB	5.24	1.60	1.54
1	D	27	THR	CA-C	5.23	1.59	1.52
1	A	250	VAL	C-O	-5.23	1.17	1.24
1	J	242	ILE	C-O	-5.14	1.18	1.24
1	C	140	ASP	N-CA	-5.09	1.40	1.46
1	L	242	ILE	C-O	5.09	1.29	1.24
1	N	72	ASP	C-O	-5.09	1.17	1.23
1	G	91	PRO	CA-C	5.04	1.58	1.52
1	G	297	LYS	CA-C	5.04	1.59	1.52
1	G	124	ILE	CA-CB	5.03	1.58	1.54
1	L	170	MET	N-CA	-5.00	1.40	1.46

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	185	GLY	N-CA-C	7.99	122.32	110.42
1	N	5	LYS	N-CA-C	7.63	121.81	110.52
1	N	237	TYR	N-CA-C	7.43	121.66	112.59
1	D	196	ARG	N-CA-C	7.04	118.95	111.28
1	P	226	GLU	N-CA-C	6.79	120.56	110.52
1	H	223	GLU	N-CA-C	6.57	119.62	107.99
1	G	136	PHE	N-CA-C	6.53	119.58	109.07
1	K	73	HIS	CA-C-N	-6.41	112.39	119.19
1	K	73	HIS	C-N-CA	-6.41	112.39	119.19
1	O	267	LEU	N-CA-C	6.34	118.19	111.28
1	E	118	ILE	CB-CA-C	-6.21	101.11	110.55
1	H	298	ASN	N-CA-C	6.17	117.82	109.24
1	A	225	ILE	CB-CA-C	-6.11	101.58	110.63
1	F	225	ILE	CB-CA-C	-6.07	101.57	110.62
1	I	99	ASN	CA-C-N	-6.06	114.15	123.17
1	I	99	ASN	C-N-CA	-6.06	114.15	123.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	187	GLU	CA-C-N	5.98	125.66	119.56
1	E	187	GLU	C-N-CA	5.98	125.66	119.56
1	C	124	ILE	CB-CA-C	-5.93	104.03	110.85
1	B	5	LYS	N-CA-C	5.91	117.68	110.41
1	M	187	GLU	CA-C-N	5.90	125.52	119.56
1	M	187	GLU	C-N-CA	5.90	125.52	119.56
1	D	252	ILE	N-CA-C	5.89	117.17	108.45
1	H	117	GLY	N-CA-C	5.86	118.84	110.46
1	B	136	PHE	N-CA-C	5.86	118.07	108.52
1	A	132	GLU	CB-CA-C	-5.82	100.96	110.85
1	J	157	ILE	N-CA-C	5.80	116.48	108.12
1	A	298	ASN	N-CA-C	5.77	117.26	109.24
1	I	298	ASN	N-CA-C	5.72	117.91	109.62
1	H	16	PHE	N-CA-C	5.67	116.03	108.38
1	I	237	TYR	N-CA-C	5.63	120.14	112.88
1	H	136	PHE	N-CA-C	5.62	118.06	108.90
1	G	157	ILE	N-CA-C	5.54	116.10	108.12
1	A	22	VAL	N-CA-C	5.54	115.74	110.42
1	O	244	GLY	CA-C-N	5.52	125.13	119.56
1	O	244	GLY	C-N-CA	5.52	125.13	119.56
1	C	237	TYR	N-CA-C	5.51	119.31	112.59
1	G	176	GLU	N-CA-C	-5.49	106.75	113.50
1	G	196	ARG	N-CA-C	5.49	116.94	111.07
1	J	196	ARG	N-CA-C	5.46	117.24	111.28
1	I	80	GLN	N-CA-C	-5.43	105.44	111.36
1	A	56	CYS	N-CA-C	5.42	119.00	112.38
1	A	92	VAL	N-CA-C	5.39	115.34	107.37
1	N	187	GLU	CA-C-N	5.37	125.04	119.56
1	N	187	GLU	C-N-CA	5.37	125.04	119.56
1	A	132	GLU	N-CA-C	5.37	117.21	111.36
1	M	35	ALA	N-CA-C	-5.33	105.55	111.36
1	K	252	ILE	N-CA-C	5.33	116.33	108.45
1	N	16	PHE	N-CA-C	5.33	116.90	108.96
1	A	68	LYS	CA-C-N	-5.32	114.30	119.78
1	A	68	LYS	C-N-CA	-5.32	114.30	119.78
1	C	252	ILE	N-CA-C	5.29	115.34	108.35
1	P	157	ILE	N-CA-C	5.29	115.51	108.11
1	N	118	ILE	N-CA-C	5.29	117.24	108.99
1	C	118	ILE	CB-CA-C	-5.27	102.53	110.55
1	I	289	LYS	N-CA-C	5.20	117.69	111.71
1	A	230	GLY	N-CA-C	5.20	125.50	113.18
1	J	187	GLU	CA-C-N	5.18	124.98	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	187	GLU	C-N-CA	5.18	124.98	119.28
1	D	193	ILE	CB-CA-C	-5.16	104.51	110.91
1	F	237	TYR	N-CA-C	5.15	119.52	112.88
1	F	244	GLY	CA-C-N	5.12	125.20	119.87
1	F	244	GLY	C-N-CA	5.12	125.20	119.87
1	L	138	PRO	CA-C-N	5.12	124.97	120.10
1	L	138	PRO	C-N-CA	5.12	124.97	120.10
1	H	259	ALA	N-CA-C	5.12	117.50	108.75
1	I	136	PHE	N-CA-C	5.09	117.20	108.90
1	P	237	TYR	N-CA-C	5.08	118.51	112.72
1	E	136	PHE	N-CA-C	5.07	117.23	109.07
1	L	73	HIS	CA-C-N	-5.06	113.83	119.19
1	L	73	HIS	C-N-CA	-5.06	113.83	119.19
1	A	289	LYS	N-CA-C	5.04	117.50	111.71
1	I	160	ASP	N-CA-C	-5.04	106.24	112.38
1	H	294	LEU	N-CA-C	-5.01	106.02	112.68
1	G	117	GLY	N-CA-C	5.00	117.14	112.04
1	N	68	LYS	CA-C-N	-5.00	114.80	119.85
1	N	68	LYS	C-N-CA	-5.00	114.80	119.85

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2347	0	2321	41	0
1	B	2372	0	2330	17	0
1	C	2390	0	2351	12	0
1	D	2372	0	2337	15	0
1	E	2357	0	2319	12	0
1	F	2368	0	2328	18	0
1	G	2344	0	2303	25	0
1	H	2248	0	2222	29	0
1	I	2318	0	2281	15	0
1	J	2368	0	2328	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	2390	0	2351	12	0
1	L	2372	0	2337	12	0
1	M	2364	0	2333	19	0
1	N	2365	0	2323	16	0
1	O	2360	0	2324	13	0
1	P	2284	0	2260	8	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	4	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	2	0
All	All	41665	0	37564	276	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 4.

All (276) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:245:PRO:HG2	1:M:273:MET:HE1	1.53	0.90
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:A:199:TRP:CD1	1:A:203[A]:MET:HE3	2.16	0.81
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:245:PRO:CG	1:M:273:MET:HE1	2.18	0.73
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:B:275[A]:HIS:HB2	6:B:686:HOH:O	2.01	0.61
1:A:199:TRP:CD1	1:A:203[A]:MET:CE	2.83	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:A:203[B]:MET:HE1	1:A:216:ALA:HB2	1.83	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:P:211:LEU:HD23	1:P:273:MET:HE3	1.85	0.58
1:I:130:TYR:HE1	6:I:690:HOH:O	1.85	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
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:125:PRO:HG3	6:A:574:HOH:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:12:SER:HA	1:E:261:LEU:O	2.07	0.54
1:A:199:TRP:NE1	1:A:203[A]:MET:HE3	2.22	0.54
1:N:245:PRO:HG2	1:N:273:MET:HE1	1.91	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:E:214:LEU:C	1:E:214:LEU:HD23	2.35	0.51
1:M:5:LYS:HD3	1:M:6:GLY:N	2.25	0.51
1:N:245:PRO:CG	1:N:273:MET:HE1	2.40	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:L:214:LEU:C	1:L:214:LEU:HD23	2.37	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:P:203:MET:HE2	6:P:567:HOH:O	2.12	0.49
1:C:285:PRO:HD2	3:C:404:EDO:H12	1.94	0.49
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:M:254:ASP:OD1	1:M:254:ASP:C	2.56	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:A:214:LEU:C	1:A:214:LEU:HD23	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:228:GLU:CD	1:I:228:GLU:H	2.21	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:48:GLU:HG2	1:A:49:LEU:HG	1.96	0.48
1:A:199:TRP:O	1:A:203[A]:MET:HE2	2.13	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:A:228:GLU:CD	1:A:228:GLU:H	2.23	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: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: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:N:245:PRO:HB2	1:N:273:MET:HE1	1.97	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:F:214:LEU:C	1:F:214:LEU:HD23	2.41	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
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:A:92:VAL:C	1:A:106:ILE:HG13	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:148:THR:O	1:G:149:LYS:C	2.60	0.45
1:H:194:ASP:C	1:H:196:ARG:H	2.25	0.45
1:C:152:LYS:HE2	6:C:552:HOH:O	2.17	0.45
1:D:254:ASP:OD1	1:D:254:ASP:C	2.60	0.45
1:O:161:GLN:CD	1:O:199:TRP:HE1	2.24	0.45
1:O:30:GLU:O	1:O:34:ARG:HG3	2.17	0.44
1:E:199:TRP:CE2	1:E:203:MET:HE1	2.53	0.44
1:I:211:LEU:HA	1:I:245:PRO:O	2.18	0.44
1:D:237:TYR:O	1:D:238:GLY:C	2.59	0.44
1:G:29:ALA:HB1	1:G:46:ILE:HD13	1.99	0.44
1:J:214:LEU:HD23	1:J:214:LEU:C	2.43	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:M:211:LEU:HD23	1:M:273:MET:HE3	1.98	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:B:214:LEU:C	1:B:214:LEU:HD23	2.43	0.43
1:F:161:GLN:CD	1:F:199:TRP:HE1	2.26	0.43
1:F:285:PRO:HD2	3:F:403:EDO:H12	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:I:203:MET:HE2	6:I:557:HOH:O	2.19	0.42
1:K:156:ALA:O	1:K:181:PRO:HD2	2.20	0.42
1:B:278:GLY:O	1:B:279:VAL:C	2.60	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:H:60:ARG:HE	1:H:62:ASP:CG	2.28	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:61:GLU:HB2	1:N:276:CYS:SG	2.60	0.42
1:N:199:TRP:CE2	1:N:203:MET:HE1	2.55	0.42
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:E:194:ASP:OD1	1:E:194:ASP:C	2.60	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:I:180:TYR:CG	1:I:203:MET:HE1	2.55	0.41
1:M:214:LEU:HD23	1:M:214:LEU:C	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:174:GLY:HA3	6:G:510:HOH:O	2.21	0.41
1:A:132:GLU:C	1:A:134:PHE:N	2.79	0.40
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
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:M:245:PRO:CB	1:M:273:MET:HE1	2.51	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

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%)	36	46
1	B	297/304 (98%)	285 (96%)	11 (4%)	1 (0%)	36	46
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%)	36	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	293/304 (96%)	281 (96%)	11 (4%)	1 (0%)	36	46
1	H	275/304 (90%)	254 (92%)	21 (8%)	0	100	100
1	I	289/304 (95%)	277 (96%)	12 (4%)	0	100	100
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%)	36	46
1	N	296/304 (97%)	286 (97%)	9 (3%)	1 (0%)	36	46
1	O	296/304 (97%)	285 (96%)	10 (3%)	1 (0%)	36	46
1	P	280/304 (92%)	271 (97%)	9 (3%)	0	100	100
All	All	4701/4864 (97%)	4520 (96%)	174 (4%)	7 (0%)	48	60

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 ⓘ

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%)	236 (96%)	11 (4%)	24	37
1	B	249/252 (99%)	241 (97%)	8 (3%)	34	51
1	C	251/252 (100%)	247 (98%)	4 (2%)	55	73
1	D	250/252 (99%)	250 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	247/252 (98%)	242 (98%)	5 (2%)	48	67
1	F	249/252 (99%)	244 (98%)	5 (2%)	48	67
1	G	246/252 (98%)	240 (98%)	6 (2%)	43	62
1	H	236/252 (94%)	225 (95%)	11 (5%)	23	35
1	I	243/252 (96%)	236 (97%)	7 (3%)	37	55
1	J	249/252 (99%)	241 (97%)	8 (3%)	34	51
1	K	251/252 (100%)	248 (99%)	3 (1%)	63	79
1	L	250/252 (99%)	249 (100%)	1 (0%)	84	92
1	M	249/252 (99%)	245 (98%)	4 (2%)	55	73
1	N	248/252 (98%)	247 (100%)	1 (0%)	84	92
1	O	248/252 (98%)	243 (98%)	5 (2%)	48	67
1	P	240/252 (95%)	229 (95%)	11 (5%)	24	36
All	All	3953/4032 (98%)	3863 (98%)	90 (2%)	44	63

All (90) 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	133	LYS
1	A	231	LYS
1	A	237	TYR
1	A	251	SER
1	B	161	GLN
1	B	211	LEU
1	B	251	SER
1	B	269	LYS
1	B	272	SER
1	B	275[A]	HIS
1	B	275[B]	HIS
1	B	297	LYS
1	C	3	GLU
1	C	4	ASP

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Mol	Chain	Res	Type
1	C	5	LYS
1	C	249	ILE
1	E	38	LYS
1	E	88	VAL
1	E	152	LYS
1	E	237	TYR
1	E	251	SER
1	F	4	ASP
1	F	5	LYS
1	F	7	ARG
1	F	214	LEU
1	F	237	TYR
1	G	8	LYS
1	G	145	VAL
1	G	149	LYS
1	G	212	VAL
1	G	256	LYS
1	G	297	LYS
1	H	5	LYS
1	H	8	LYS
1	H	19	THR
1	H	28	THR
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	61	GLU
1	I	88	VAL
1	I	130	TYR
1	I	222	ASN
1	I	232	SER
1	I	237	TYR
1	I	297	LYS
1	J	4	ASP
1	J	5	LYS
1	J	211	LEU
1	J	251	SER
1	J	252	ILE
1	J	281	ARG

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Mol	Chain	Res	Type
1	J	297	LYS
1	J	301	LEU
1	K	4	ASP
1	K	269	LYS
1	K	297	LYS
1	L	297	LYS
1	M	5	LYS
1	M	118	ILE
1	M	161	GLN
1	M	251	SER
1	N	256	LYS
1	O	5	LYS
1	O	108	ILE
1	O	118	ILE
1	O	161	GLN
1	O	269	LYS
1	P	5	LYS
1	P	71	LYS
1	P	81	LYS
1	P	88	VAL
1	P	118	ILE
1	P	126	ASP
1	P	133	LYS
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 (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	HIS
1	A	59	GLN
1	A	100	ASN
1	A	161	GLN
1	A	204	GLN
1	B	59	GLN
1	C	65	GLN
1	C	191	GLN
1	C	229	HIS
1	C	298	ASN
1	D	204	GLN

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Mol	Chain	Res	Type
1	D	222	ASN
1	D	239	ASN
1	E	65	GLN
1	E	204	GLN
1	E	222	ASN
1	F	65	GLN
1	F	204	GLN
1	F	222	ASN
1	G	59	GLN
1	G	102	HIS
1	G	189	HIS
1	G	204	GLN
1	G	229	HIS
1	H	161	GLN
1	H	204	GLN
1	H	222	ASN
1	I	102	HIS
1	I	137	ASN
1	I	161	GLN
1	I	204	GLN
1	I	222	ASN
1	J	65	GLN
1	J	204	GLN
1	K	65	GLN
1	K	298	ASN
1	L	65	GLN
1	L	222	ASN
1	M	59	GLN
1	M	204	GLN
1	N	65	GLN
1	N	204	GLN
1	O	39	GLN
1	O	59	GLN
1	O	65	GLN
1	O	102	HIS
1	O	189	HIS
1	P	39	GLN
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 oligosaccharides 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	K	404	-	5,5,5	0.54	0	5,5,5	0.27	0
2	GOL	I	401	-	5,5,5	0.48	0	5,5,5	0.16	0
2	GOL	O	402	-	5,5,5	0.26	0	5,5,5	0.73	0
3	EDO	P	403	-	3,3,3	0.50	0	2,2,2	0.34	0
3	EDO	A	403	-	3,3,3	0.48	0	2,2,2	0.36	0
2	GOL	J	404	-	5,5,5	0.34	0	5,5,5	0.33	0
2	GOL	N	404	-	5,5,5	0.48	0	5,5,5	0.24	0
5	PEG	K	406	-	6,6,6	0.60	0	5,5,5	0.14	0
2	GOL	E	403	-	5,5,5	0.50	0	5,5,5	0.45	0
4	PUT	M	401	-	5,5,5	0.47	0	4,4,4	0.67	0
4	PUT	N	402	-	5,5,5	0.27	0	4,4,4	0.60	0
4	PUT	D	402	-	5,5,5	0.21	0	4,4,4	0.81	0
2	GOL	N	401	-	5,5,5	0.24	0	5,5,5	0.25	0
3	EDO	I	402	-	3,3,3	0.62	0	2,2,2	0.11	0
5	PEG	D	406	-	6,6,6	0.69	0	5,5,5	0.18	0
2	GOL	G	403	-	5,5,5	0.48	0	5,5,5	0.25	0
3	EDO	I	403	-	3,3,3	0.48	0	2,2,2	0.46	0
2	GOL	K	403	-	5,5,5	0.68	0	5,5,5	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	K	405	-	3,3,3	0.56	0	2,2,2	0.16	0
4	PUT	B	401	-	5,5,5	0.34	0	4,4,4	0.77	0
2	GOL	L	402	-	5,5,5	0.81	0	5,5,5	0.52	0
2	GOL	C	403	-	5,5,5	0.53	0	5,5,5	0.42	0
2	GOL	J	403	-	5,5,5	0.59	0	5,5,5	0.73	0
2	GOL	N	405	-	5,5,5	0.68	0	5,5,5	0.53	0
3	EDO	N	406	-	3,3,3	0.57	0	2,2,2	0.05	0
3	EDO	F	403	-	3,3,3	0.58	0	2,2,2	0.23	0
2	GOL	P	401	-	5,5,5	0.45	0	5,5,5	0.15	0
4	PUT	L	401	-	5,5,5	0.43	0	4,4,4	0.78	0
3	EDO	B	404	-	3,3,3	0.57	0	2,2,2	0.19	0
5	PEG	L	405	-	6,6,6	0.59	0	5,5,5	0.34	0
3	EDO	M	403	-	3,3,3	0.74	0	2,2,2	0.07	0
2	GOL	J	402	-	5,5,5	0.39	0	5,5,5	0.41	0
4	PUT	C	401	-	5,5,5	0.26	0	4,4,4	0.93	0
2	GOL	F	402	-	5,5,5	0.53	0	5,5,5	0.23	0
3	EDO	C	404	-	3,3,3	0.66	0	2,2,2	0.34	0
2	GOL	N	403	-	5,5,5	0.81	0	5,5,5	0.67	0
2	GOL	B	402	-	5,5,5	0.71	0	5,5,5	0.61	0
2	GOL	G	402	-	5,5,5	0.46	0	5,5,5	0.61	0
3	EDO	F	404	-	3,3,3	0.55	0	2,2,2	0.32	0
3	EDO	L	403	-	3,3,3	0.50	0	2,2,2	0.29	0
2	GOL	D	401	-	5,5,5	0.43	0	5,5,5	0.32	0
4	PUT	G	401	-	5,5,5	0.22	0	4,4,4	1.12	1 (25%)
4	PUT	O	401	-	5,5,5	0.34	0	4,4,4	0.80	0
4	PUT	F	401	-	5,5,5	0.35	0	4,4,4	0.45	0
2	GOL	C	402	-	5,5,5	0.44	0	5,5,5	0.51	0
4	PUT	K	401	-	5,5,5	0.37	0	4,4,4	0.62	0
2	GOL	A	401	-	5,5,5	0.61	0	5,5,5	0.67	0
3	EDO	D	404	-	3,3,3	0.59	0	2,2,2	0.23	0
2	GOL	E	404	-	5,5,5	0.37	0	5,5,5	0.34	0
4	PUT	J	401	-	5,5,5	0.41	0	4,4,4	0.99	0
3	EDO	L	404	-	3,3,3	0.51	0	2,2,2	0.16	0
3	EDO	D	405	-	3,3,3	0.47	0	2,2,2	0.39	0
3	EDO	B	405	-	3,3,3	0.65	0	2,2,2	0.08	0
2	GOL	B	403	-	5,5,5	0.31	0	5,5,5	0.40	0
2	GOL	K	402	-	5,5,5	0.63	0	5,5,5	0.44	0
2	GOL	E	402	-	5,5,5	0.39	0	5,5,5	0.40	0
2	GOL	A	402	-	5,5,5	0.49	0	5,5,5	0.24	0
2	GOL	D	403	-	5,5,5	0.83	0	5,5,5	0.53	0
2	GOL	E	405	-	5,5,5	0.60	0	5,5,5	0.44	0
2	GOL	M	402	-	5,5,5	0.41	0	5,5,5	0.22	0
3	EDO	P	402	-	3,3,3	0.56	0	2,2,2	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PUT	E	401	-	5,5,5	0.20	0	4,4,4	0.84	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	K	404	-	-	4/4/4/4	-
2	GOL	I	401	-	-	2/4/4/4	-
2	GOL	O	402	-	-	3/4/4/4	-
3	EDO	P	403	-	-	1/1/1/1	-
3	EDO	A	403	-	-	1/1/1/1	-
2	GOL	J	404	-	-	3/4/4/4	-
2	GOL	N	404	-	-	1/4/4/4	-
5	PEG	K	406	-	-	3/4/4/4	-
2	GOL	E	403	-	-	2/4/4/4	-
4	PUT	M	401	-	-	0/3/3/3	-
4	PUT	N	402	-	-	0/3/3/3	-
4	PUT	D	402	-	-	0/3/3/3	-
2	GOL	N	401	-	-	2/4/4/4	-
3	EDO	I	402	-	-	1/1/1/1	-
5	PEG	D	406	-	-	1/4/4/4	-
2	GOL	G	403	-	-	4/4/4/4	-
3	EDO	I	403	-	-	0/1/1/1	-
2	GOL	K	403	-	-	4/4/4/4	-
3	EDO	K	405	-	-	1/1/1/1	-
4	PUT	B	401	-	-	0/3/3/3	-
2	GOL	L	402	-	-	4/4/4/4	-
2	GOL	C	403	-	-	4/4/4/4	-
2	GOL	J	403	-	-	2/4/4/4	-
2	GOL	N	405	-	-	4/4/4/4	-
3	EDO	N	406	-	-	0/1/1/1	-
3	EDO	F	403	-	-	1/1/1/1	-
2	GOL	P	401	-	-	4/4/4/4	-
4	PUT	L	401	-	-	0/3/3/3	-
3	EDO	B	404	-	-	1/1/1/1	-
5	PEG	L	405	-	-	2/4/4/4	-
3	EDO	M	403	-	-	1/1/1/1	-

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	401	PUT	C2-C3-C4	-2.05	99.39	113.42

There are no chirality outliers.

All (99) 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	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
2	M	402	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
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
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
5	K	406	PEG	O1-C1-C2-O2
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
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	A	402	GOL	C1-C2-C3-O3
5	K	406	PEG	O2-C3-C4-O4
3	A	403	EDO	O1-C1-C2-O2
3	B	404	EDO	O1-C1-C2-O2
2	A	401	GOL	O1-C1-C2-O2
2	C	403	GOL	O1-C1-C2-O2
3	K	405	EDO	O1-C1-C2-O2
3	P	402	EDO	O1-C1-C2-O2
2	C	403	GOL	O2-C2-C3-O3
2	E	402	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	K	403	GOL	O1-C1-C2-O2
2	O	402	GOL	O1-C1-C2-C3
5	L	405	PEG	O1-C1-C2-O2
2	D	403	GOL	O2-C2-C3-O3
2	N	403	GOL	O1-C1-C2-C3
3	F	404	EDO	O1-C1-C2-O2
2	L	402	GOL	O1-C1-C2-O2
5	D	406	PEG	O1-C1-C2-O2
2	P	401	GOL	O1-C1-C2-O2
2	P	401	GOL	O2-C2-C3-O3
3	I	402	EDO	O1-C1-C2-O2
5	K	406	PEG	C4-C3-O2-C2
2	A	402	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	A	403	EDO	2	0
3	I	402	EDO	1	0
3	K	405	EDO	1	0
2	L	402	GOL	4	0
2	C	403	GOL	1	0
3	F	403	EDO	1	0
3	C	404	EDO	2	0
3	L	403	EDO	2	0
2	D	401	GOL	1	0
4	K	401	PUT	1	0
2	A	401	GOL	2	0
3	D	404	EDO	1	0
3	B	405	EDO	1	0
2	B	403	GOL	1	0
2	K	402	GOL	1	0
2	D	403	GOL	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	295/304 (97%)	-0.12	14 (4%) 36 38	23, 45, 95, 132	2 (0%)
1	B	298/304 (98%)	-0.56	1 (0%) 90 90	25, 36, 59, 115	1 (0%)
1	C	301/304 (99%)	-0.64	3 (0%) 79 80	23, 35, 54, 112	1 (0%)
1	D	298/304 (98%)	-0.72	0 100 100	18, 33, 49, 92	2 (0%)
1	E	297/304 (97%)	-0.61	1 (0%) 90 90	26, 37, 57, 92	0
1	F	298/304 (98%)	-0.40	1 (0%) 90 90	25, 44, 64, 93	1 (0%)
1	G	295/304 (97%)	0.58	10 (3%) 48 50	47, 65, 84, 101	0
1	H	282/304 (92%)	1.24	52 (18%) 3 4	39, 85, 118, 136	1 (0%)
1	I	292/304 (96%)	-0.31	5 (1%) 69 70	26, 41, 84, 138	1 (0%)
1	J	298/304 (98%)	-0.57	0 100 100	26, 36, 58, 118	1 (0%)
1	K	301/304 (99%)	-0.62	2 (0%) 84 85	24, 37, 59, 111	1 (0%)
1	L	298/304 (98%)	-0.73	0 100 100	24, 34, 50, 91	2 (0%)
1	M	297/304 (97%)	-0.67	1 (0%) 90 90	25, 35, 52, 88	2 (0%)
1	N	298/304 (98%)	-0.65	0 100 100	25, 35, 52, 92	0
1	O	297/304 (97%)	-0.31	1 (0%) 90 90	32, 46, 66, 108	1 (0%)
1	P	287/304 (94%)	0.31	12 (4%) 40 42	27, 61, 104, 119	1 (0%)
All	All	4732/4864 (97%)	-0.31	103 (2%) 62 64	18, 40, 87, 138	17 (0%)

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	127	GLY	5.3
1	P	227	THR	4.8
1	A	193	ILE	4.6
1	H	224	ILE	4.3
1	P	188	PRO	4.3

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Mol	Chain	Res	Type	RSRZ
1	H	225	ILE	4.3
1	A	130	TYR	4.2
1	H	130	TYR	4.1
1	A	301	LEU	4.0
1	P	193	ILE	3.9
1	A	128	PRO	3.8
1	H	227	THR	3.7
1	H	234	ILE	3.6
1	P	130	TYR	3.6
1	H	185	GLY	3.6
1	H	74	PRO	3.4
1	G	8	LYS	3.4
1	H	58	ALA	3.3
1	H	76	ILE	3.3
1	H	300	VAL	3.2
1	H	5	LYS	3.2
1	F	301	LEU	3.2
1	G	273	MET	3.2
1	P	5	LYS	3.1
1	I	130	TYR	3.0
1	A	129	GLY	3.0
1	C	1	MET	3.0
1	H	22	VAL	2.9
1	H	71	LYS	2.9
1	H	187	GLU	2.9
1	H	94	PHE	2.8
1	H	232	SER	2.8
1	C	2	ALA	2.8
1	O	5	LYS	2.8
1	I	128	PRO	2.7
1	H	118	ILE	2.7
1	K	1	MET	2.7
1	G	279	VAL	2.6
1	K	2	ALA	2.6
1	I	188	PRO	2.6
1	B	275[A]	HIS	2.6
1	I	129	GLY	2.6
1	H	23	SER	2.6
1	A	5	LYS	2.5
1	H	64	ILE	2.5
1	H	226	GLU	2.5
1	H	19	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	I	300	VAL	2.5
1	H	17	ALA	2.5
1	H	21	ASP	2.5
1	A	229	HIS	2.5
1	H	98	ALA	2.5
1	A	188	PRO	2.5
1	G	76	ILE	2.4
1	H	49	LEU	2.4
1	G	89	VAL	2.4
1	P	300	VAL	2.4
1	H	24	THR	2.4
1	H	55	PHE	2.4
1	H	66	ARG	2.3
1	H	195	SER	2.3
1	H	273	MET	2.3
1	P	58	ALA	2.3
1	H	57	GLN	2.3
1	H	124	ILE	2.3
1	H	99	ASN	2.3
1	H	53	TYR	2.3
1	H	220	ILE	2.3
1	C	301	LEU	2.2
1	A	230	GLY	2.2
1	H	77	MET	2.2
1	A	58	ALA	2.2
1	H	70	TYR	2.2
1	E	301	LEU	2.2
1	G	260	VAL	2.2
1	H	50	PHE	2.2
1	H	65	GLN	2.2
1	H	186	SER	2.2
1	H	75	THR	2.2
1	P	101	ALA	2.2
1	H	46	ILE	2.2
1	H	86	LEU	2.1
1	H	294	LEU	2.1
1	P	256	LYS	2.1
1	G	22	VAL	2.1
1	H	92	VAL	2.1
1	G	301	LEU	2.1
1	H	299	PRO	2.1
1	A	133	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	101	ALA	2.1
1	G	82	LEU	2.1
1	H	233	GLU	2.0
1	P	57	GLN	2.0
1	P	100	ASN	2.0
1	H	184	ILE	2.0
1	H	26	VAL	2.0
1	H	159	TRP	2.0
1	A	192	SER	2.0
1	H	28	THR	2.0
1	G	107	ALA	2.0
1	A	100	ASN	2.0
1	M	301	LEU	2.0
1	A	231	LYS	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	EDO	B	404	4/4	0.81	0.18	71,72,89,91	0
3	EDO	P	402	4/4	0.81	0.17	69,80,85,86	0
3	EDO	L	404	4/4	0.83	0.18	70,78,84,85	0
2	GOL	J	403	6/6	0.84	0.17	62,64,74,80	0
2	GOL	A	402	6/6	0.84	0.16	59,66,75,98	0
2	GOL	P	401	6/6	0.86	0.15	75,79,82,83	0
3	EDO	B	405	4/4	0.86	0.19	49,62,74,83	0
2	GOL	N	405	6/6	0.87	0.16	62,69,85,89	0
2	GOL	E	405	6/6	0.88	0.14	71,83,91,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	F	404	4/4	0.88	0.15	71,72,75,79	0
2	GOL	F	402	6/6	0.89	0.14	57,66,70,71	0
2	GOL	D	403	6/6	0.89	0.14	48,60,69,72	0
3	EDO	D	405	4/4	0.89	0.15	69,75,75,80	0
5	PEG	D	406	7/7	0.89	0.16	57,72,84,89	0
5	PEG	L	405	7/7	0.89	0.13	62,68,83,83	0
2	GOL	G	402	6/6	0.90	0.15	79,88,91,94	0
2	GOL	J	404	6/6	0.90	0.14	61,73,77,80	0
5	PEG	K	406	7/7	0.90	0.15	52,81,94,96	0
2	GOL	G	403	6/6	0.90	0.14	46,60,62,65	0
3	EDO	K	405	4/4	0.91	0.15	51,59,62,63	0
3	EDO	L	403	4/4	0.91	0.15	59,59,63,63	0
3	EDO	D	404	4/4	0.91	0.18	62,65,75,75	0
2	GOL	A	401	6/6	0.91	0.13	55,74,75,75	0
3	EDO	P	403	4/4	0.91	0.19	75,77,79,80	0
3	EDO	F	403	4/4	0.91	0.15	54,63,64,73	0
2	GOL	L	402	6/6	0.91	0.11	45,55,58,59	0
3	EDO	I	403	4/4	0.91	0.20	55,82,83,85	0
2	GOL	K	404	6/6	0.92	0.13	53,58,64,71	0
4	PUT	G	401	6/6	0.92	0.15	66,68,72,76	0
2	GOL	B	403	6/6	0.92	0.13	53,67,70,73	0
3	EDO	M	403	4/4	0.92	0.16	62,65,71,71	0
2	GOL	E	402	6/6	0.92	0.14	51,64,78,84	0
2	GOL	O	402	6/6	0.93	0.11	59,64,68,73	0
2	GOL	E	403	6/6	0.93	0.15	62,71,87,99	0
4	PUT	J	401	6/6	0.93	0.09	38,40,42,43	0
3	EDO	C	404	4/4	0.93	0.13	52,57,63,63	0
3	EDO	I	402	4/4	0.93	0.15	53,58,60,69	0
3	EDO	A	403	4/4	0.93	0.13	52,61,61,65	0
2	GOL	N	403	6/6	0.94	0.11	44,58,71,75	0
2	GOL	E	404	6/6	0.94	0.10	49,54,60,61	0
4	PUT	K	401	6/6	0.94	0.12	41,42,45,45	0
2	GOL	I	401	6/6	0.94	0.10	54,60,69,70	0
2	GOL	C	403	6/6	0.94	0.12	43,57,66,67	0
4	PUT	B	401	6/6	0.94	0.10	39,40,40,40	0
3	EDO	N	406	4/4	0.95	0.13	57,58,64,65	0
2	GOL	N	404	6/6	0.95	0.10	44,51,60,61	0
2	GOL	M	402	6/6	0.95	0.10	44,54,70,70	0
4	PUT	L	401	6/6	0.95	0.11	41,45,50,50	0
4	PUT	M	401	6/6	0.95	0.09	34,35,37,39	0
4	PUT	N	402	6/6	0.95	0.10	47,47,49,51	0
4	PUT	O	401	6/6	0.95	0.10	47,48,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	B	402	6/6	0.95	0.10	49,55,62,67	0
4	PUT	E	401	6/6	0.95	0.10	36,37,43,45	0
4	PUT	F	401	6/6	0.95	0.12	59,62,67,67	0
2	GOL	N	401	6/6	0.96	0.09	46,58,69,73	0
2	GOL	K	402	6/6	0.96	0.12	48,59,59,69	0
2	GOL	K	403	6/6	0.96	0.10	45,52,63,67	0
2	GOL	J	402	6/6	0.96	0.09	45,52,58,66	0
2	GOL	D	401	6/6	0.96	0.10	49,57,75,78	0
2	GOL	C	402	6/6	0.96	0.09	45,52,69,77	0
4	PUT	C	401	6/6	0.97	0.09	36,38,41,44	0
4	PUT	D	402	6/6	0.97	0.09	37,41,44,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.