



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 27, 2017 – 12:42 AM EDT

PDB ID : 4CMB
Title : Crystal structure of pteridine reductase 1 (PTR1) from Trypanosoma brucei
in ternary complex with cofactor and inhibitor
Authors : Barrack, K.L.; Hunter, W.N.
Deposited on : 2014-01-16
Resolution : 1.96 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029077
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029077

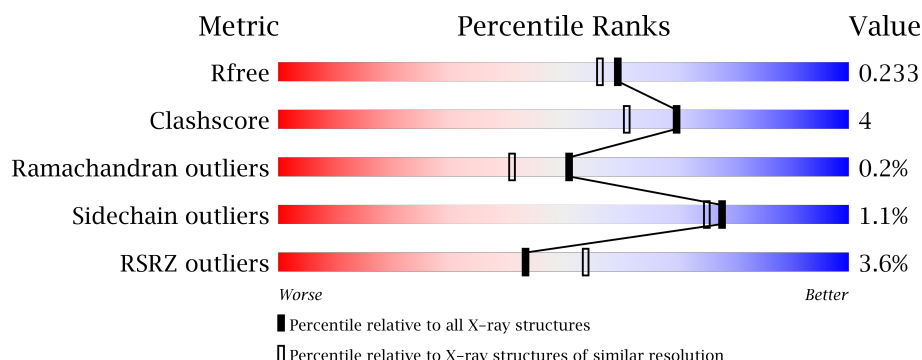
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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}	100719	2004 (1.96-1.96)
Clashscore	112137	2136 (1.96-1.96)
Ramachandran outliers	110173	2117 (1.96-1.96)
Sidechain outliers	110143	2117 (1.96-1.96)
RSRZ outliers	101464	2018 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	288	<div> <div>4%</div> <div> <div></div> <div>79%</div> <div>8%</div> <div>13%</div> </div> </div>
1	B	288	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>7%</div> <div>13%</div> </div> </div>
1	C	288	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>11%</div> <div>14%</div> </div> </div>
1	D	288	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>8%</div> <div>14%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8567 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 PTERIDINE REDUCTASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	251	Total	C	N	O	S	0	7	0
			1907	1199	335	362	11			
1	B	250	Total	C	N	O	S	0	1	0
			1868	1174	329	353	12			
1	C	249	Total	C	N	O	S	0	3	0
			1867	1176	327	352	12			
1	D	249	Total	C	N	O	S	0	2	0
			1866	1173	328	354	11			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP O76290
A	-18	GLY	-	expression tag	UNP O76290
A	-17	SER	-	expression tag	UNP O76290
A	-16	SER	-	expression tag	UNP O76290
A	-15	HIS	-	expression tag	UNP O76290
A	-14	HIS	-	expression tag	UNP O76290
A	-13	HIS	-	expression tag	UNP O76290
A	-12	HIS	-	expression tag	UNP O76290
A	-11	HIS	-	expression tag	UNP O76290
A	-10	HIS	-	expression tag	UNP O76290
A	-9	SER	-	expression tag	UNP O76290
A	-8	SER	-	expression tag	UNP O76290
A	-7	GLY	-	expression tag	UNP O76290
A	-6	LEU	-	expression tag	UNP O76290
A	-5	VAL	-	expression tag	UNP O76290
A	-4	PRO	-	expression tag	UNP O76290
A	-3	ARG	-	expression tag	UNP O76290
A	-2	GLY	-	expression tag	UNP O76290
A	-1	SER	-	expression tag	UNP O76290
A	0	HIS	-	expression tag	UNP O76290
B	-19	MET	-	expression tag	UNP O76290

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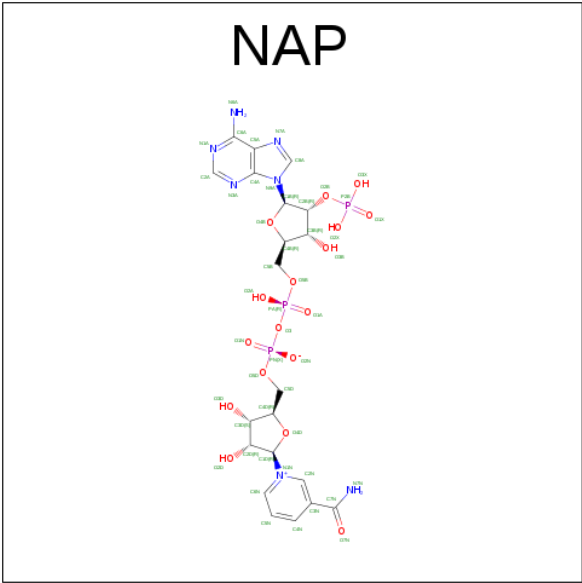
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP O76290
B	-17	SER	-	expression tag	UNP O76290
B	-16	SER	-	expression tag	UNP O76290
B	-15	HIS	-	expression tag	UNP O76290
B	-14	HIS	-	expression tag	UNP O76290
B	-13	HIS	-	expression tag	UNP O76290
B	-12	HIS	-	expression tag	UNP O76290
B	-11	HIS	-	expression tag	UNP O76290
B	-10	HIS	-	expression tag	UNP O76290
B	-9	SER	-	expression tag	UNP O76290
B	-8	SER	-	expression tag	UNP O76290
B	-7	GLY	-	expression tag	UNP O76290
B	-6	LEU	-	expression tag	UNP O76290
B	-5	VAL	-	expression tag	UNP O76290
B	-4	PRO	-	expression tag	UNP O76290
B	-3	ARG	-	expression tag	UNP O76290
B	-2	GLY	-	expression tag	UNP O76290
B	-1	SER	-	expression tag	UNP O76290
B	0	HIS	-	expression tag	UNP O76290
C	-19	MET	-	expression tag	UNP O76290
C	-18	GLY	-	expression tag	UNP O76290
C	-17	SER	-	expression tag	UNP O76290
C	-16	SER	-	expression tag	UNP O76290
C	-15	HIS	-	expression tag	UNP O76290
C	-14	HIS	-	expression tag	UNP O76290
C	-13	HIS	-	expression tag	UNP O76290
C	-12	HIS	-	expression tag	UNP O76290
C	-11	HIS	-	expression tag	UNP O76290
C	-10	HIS	-	expression tag	UNP O76290
C	-9	SER	-	expression tag	UNP O76290
C	-8	SER	-	expression tag	UNP O76290
C	-7	GLY	-	expression tag	UNP O76290
C	-6	LEU	-	expression tag	UNP O76290
C	-5	VAL	-	expression tag	UNP O76290
C	-4	PRO	-	expression tag	UNP O76290
C	-3	ARG	-	expression tag	UNP O76290
C	-2	GLY	-	expression tag	UNP O76290
C	-1	SER	-	expression tag	UNP O76290
C	0	HIS	-	expression tag	UNP O76290
D	-19	MET	-	expression tag	UNP O76290
D	-18	GLY	-	expression tag	UNP O76290
D	-17	SER	-	expression tag	UNP O76290

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP O76290
D	-15	HIS	-	expression tag	UNP O76290
D	-14	HIS	-	expression tag	UNP O76290
D	-13	HIS	-	expression tag	UNP O76290
D	-12	HIS	-	expression tag	UNP O76290
D	-11	HIS	-	expression tag	UNP O76290
D	-10	HIS	-	expression tag	UNP O76290
D	-9	SER	-	expression tag	UNP O76290
D	-8	SER	-	expression tag	UNP O76290
D	-7	GLY	-	expression tag	UNP O76290
D	-6	LEU	-	expression tag	UNP O76290
D	-5	VAL	-	expression tag	UNP O76290
D	-4	PRO	-	expression tag	UNP O76290
D	-3	ARG	-	expression tag	UNP O76290
D	-2	GLY	-	expression tag	UNP O76290
D	-1	SER	-	expression tag	UNP O76290
D	0	HIS	-	expression tag	UNP O76290

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



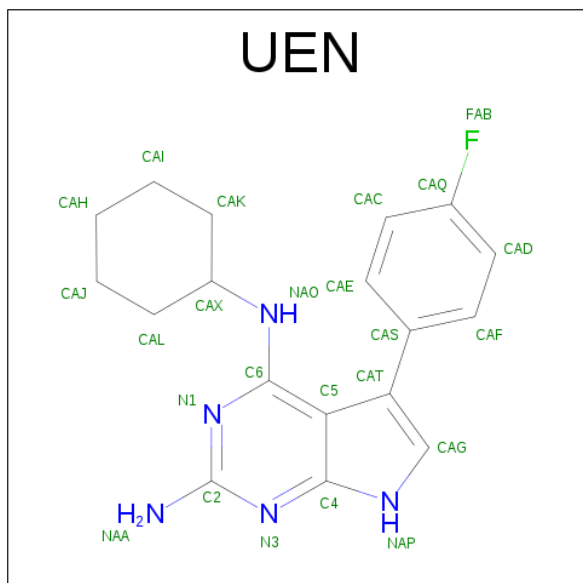
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	B	1	Total 48	C 21	N 7	O 17	P 3	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is N4-cyclohexyl-5-(4-fluorophenyl)-7H-pyrrolo[2,3-d]pyrimidine-2,4-diamine (three-letter code: UEN) (formula: C₁₈H₂₀FN₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	F	N	0	0
			24	18	1	5		
3	B	1	Total	C	F	N	0	0
			24	18	1	5		
3	C	1	Total	C	F	N	0	0
			24	18	1	5		
3	D	1	Total	C	F	N	0	0
			24	18	1	5		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

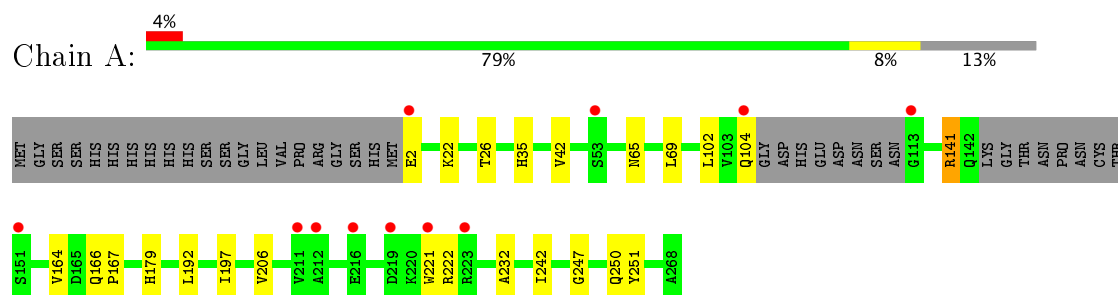
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	230	Total	O	0	0
			230	230		
5	B	201	Total	O	0	0
			201	201		
5	C	181	Total	O	0	0
			181	181		
5	D	155	Total	O	0	0
			155	155		

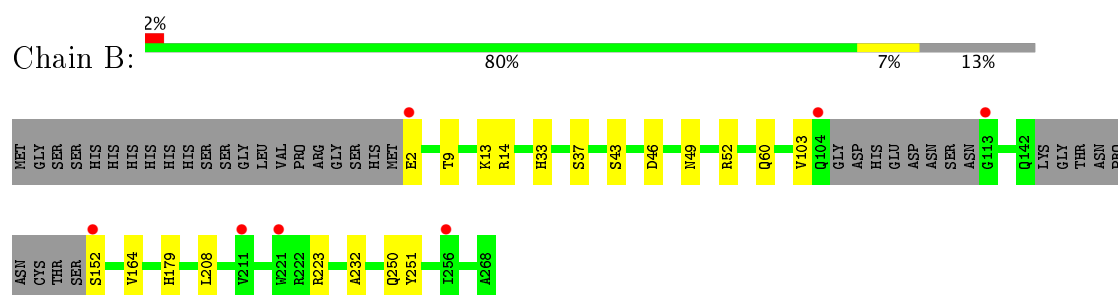
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

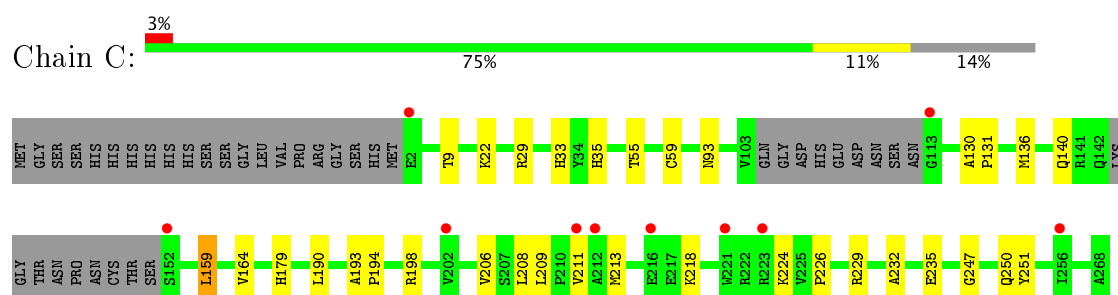
• Molecule 1: PTERIDINE REDUCTASE 1



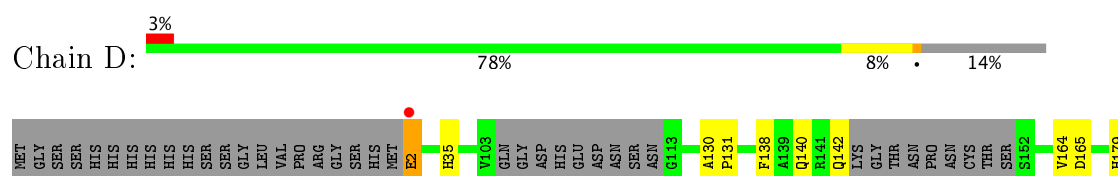
• Molecule 1: PTERIDINE REDUCTASE 1

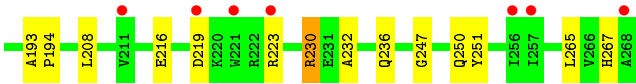


• Molecule 1: PTERIDINE REDUCTASE 1



• Molecule 1: PTERIDINE REDUCTASE 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.06 Å 89.68 Å 84.35 Å 90.00° 115.44° 90.00°	Depositor
Resolution (Å)	37.50 – 1.96 37.80 – 2.00	Depositor EDS
% Data completeness (in resolution range)	91.1 (37.50-1.96) 99.3 (37.80-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.36 (at 2.00 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.172 , 0.223 0.184 , 0.233	Depositor DCC
R_{free} test set	3374 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	15.7	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8567	wwPDB-VP
Average B, all atoms (Å ²)	19.0	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 21.43 % 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 7.0319e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: NAP, UEN, ACT

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	0.72	0/1949	0.80	0/2643
1	B	0.73	0/1898	0.80	1/2574 (0.0%)
1	C	0.70	0/1903	0.81	2/2581 (0.1%)
1	D	0.73	0/1899	0.83	4/2576 (0.2%)
All	All	0.72	0/7649	0.81	7/10374 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	230	ARG	NE-CZ-NH1	7.80	124.20	120.30
1	D	230	ARG	NE-CZ-NH2	-7.64	116.48	120.30
1	C	159	LEU	CA-CB-CG	-7.43	98.20	115.30
1	D	165	ASP	CB-CG-OD2	-7.25	111.78	118.30
1	C	198	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	B	46	ASP	CB-CG-OD1	5.74	123.47	118.30
1	D	165	ASP	CB-CG-OD1	5.22	123.00	118.30

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	1907	0	1943	18	0
1	B	1868	0	1894	12	0
1	C	1867	0	1902	25	0
1	D	1866	0	1891	17	0
2	A	48	0	25	1	0
2	B	48	0	25	0	0
2	C	48	0	25	1	0
2	D	48	0	25	1	0
3	A	24	0	20	1	0
3	B	24	0	20	2	0
3	C	24	0	20	0	0
3	D	24	0	20	0	0
4	A	4	0	3	1	0
5	A	230	0	0	9	0
5	B	201	0	0	3	0
5	C	181	0	0	2	0
5	D	155	0	0	1	0
All	All	8567	0	7813	65	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 (65) 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:167:PRO:HG2	1:C:190[B]:LEU:HD12	1.68	0.76
1:D:164:VAL:HG22	1:D:179:HIS:CD2	2.22	0.74
1:B:103:VAL:HA	1:D:140[B]:GLN:HE22	1.53	0.72
5:A:2132:HOH:O	1:C:140:GLN:NE2	2.22	0.71
1:A:206[B]:VAL:HG11	1:A:221:TRP:CE3	2.29	0.68
1:D:230:ARG:HH22	1:D:236:GLN:HE22	1.41	0.68
1:A:250:GLN:HG3	5:A:2206:HOH:O	1.93	0.67
1:A:164:VAL:HG22	1:A:179:HIS:CD2	2.33	0.63
1:D:219:ASP:OD2	1:D:223:ARG:NH1	2.33	0.62
1:D:2:GLU:HB3	5:D:2001:HOH:O	1.99	0.61
1:A:26:THR:O	1:A:26:THR:HG22	2.01	0.60
1:B:250:GLN:HG3	5:B:2186:HOH:O	2.02	0.60
5:A:2166:HOH:O	1:C:179:HIS:ND1	2.20	0.59
5:A:2164:HOH:O	1:D:267:HIS:NE2	2.32	0.57
1:A:42:VAL:HG23	5:A:2053:HOH:O	2.03	0.56
1:A:141:ARG:HG3	5:A:2106:HOH:O	2.05	0.55
1:D:247:GLY:O	1:D:250:GLN:HG2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:LYS:HE2	1:B:37:SER:OG	2.06	0.54
1:B:103:VAL:HA	1:D:140[B]:GLN:NE2	2.23	0.53
1:D:140[B]:GLN:HA	1:D:140[B]:GLN:HE21	1.75	0.52
1:C:190[B]:LEU:HD21	1:D:265:LEU:HB2	1.91	0.52
1:C:251:TYR:CE2	1:D:232:ALA:HB2	2.44	0.51
1:A:247:GLY:O	1:A:250:GLN:HG2	2.11	0.51
1:D:138:PHE:O	1:D:142:GLN:HG2	2.12	0.50
1:A:104:GLN:H	1:C:140:GLN:HE22	1.60	0.50
1:C:206:VAL:HG21	1:C:209:LEU:HD11	1.94	0.50
1:A:42:VAL:CG2	5:A:2053:HOH:O	2.57	0.49
1:C:35:HIS:HB2	2:C:1269:NAP:C2A	2.43	0.49
1:A:65:ASN:HA	1:A:69:LEU:HD22	1.94	0.49
1:B:60:GLN:OE1	5:B:2063:HOH:O	2.19	0.49
1:C:224:LYS:O	1:C:226:PRO:HD3	2.13	0.48
1:A:232:ALA:HB2	1:B:251:TYR:CE2	2.49	0.47
1:D:130:ALA:HB3	1:D:131:PRO:HD3	1.97	0.46
1:C:93:ASN:HB2	1:C:159:LEU:HD13	1.98	0.46
1:D:193:ALA:N	1:D:194:PRO:CD	2.78	0.46
1:B:9:THR:HA	1:B:33:HIS:HB3	1.97	0.46
1:C:193:ALA:N	1:C:194:PRO:CD	2.79	0.45
1:A:22:LYS:HG2	1:A:242:ILE:HG13	1.97	0.45
1:A:251:TYR:CE2	1:B:232:ALA:HB2	2.52	0.45
1:C:232:ALA:HB2	1:D:251:TYR:CE2	2.51	0.45
1:C:164:VAL:HG22	1:C:179:HIS:CD2	2.52	0.45
3:B:1270:UEN:HAO	3:B:1270:UEN:CAF	2.30	0.45
1:B:164:VAL:HG22	1:B:179:HIS:CD2	2.51	0.45
1:B:49:ASN:HA	1:B:52:ARG:O	2.17	0.45
1:C:213:MET:HG2	1:C:218:LYS:HG3	1.98	0.44
1:B:223:ARG:NH2	5:B:2168:HOH:O	2.44	0.44
1:C:22:LYS:HE2	1:C:235:GLU:HG3	2.00	0.44
1:C:206:VAL:CG2	1:C:209:LEU:HD11	2.48	0.44
1:C:9:THR:HA	1:C:33:HIS:HB3	2.00	0.43
1:C:229:ARG:NH2	5:C:2144:HOH:O	2.53	0.42
1:C:29:ARG:HG2	1:C:55:THR:HG22	2.02	0.42
3:A:1270:UEN:CAE	3:A:1270:UEN:HAO	2.33	0.42
1:C:247:GLY:O	1:C:250:GLN:HG2	2.19	0.42
1:D:35:HIS:HB2	2:D:1269:NAP:C2A	2.49	0.42
4:A:1271:ACT:H1	5:A:2229:HOH:O	2.20	0.42
1:A:102:LEU:O	1:C:136[B]:MET:HG3	2.21	0.41
1:C:33:HIS:HA	1:C:59:CYS:O	2.20	0.41
1:B:14:ARG:NH2	3:B:1270:UEN:HAL2	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:LYS:CE	1:C:235:GLU:HG3	2.50	0.41
1:C:208:LEU:HD11	5:C:2149:HOH:O	2.21	0.41
1:D:164:VAL:HG22	1:D:179:HIS:NE2	2.36	0.41
1:A:192:LEU:HB3	1:A:197:ILE:HB	2.02	0.40
1:A:35:HIS:HB2	2:A:1269:NAP:C2A	2.51	0.40
1:A:222:ARG:HD2	5:A:2191:HOH:O	2.21	0.40
1:C:130:ALA:HB3	1:C:131:PRO:HD3	2.03	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	252/288 (88%)	241 (96%)	11 (4%)	0	100	100
1	B	245/288 (85%)	237 (97%)	7 (3%)	1 (0%)	38	25
1	C	246/288 (85%)	236 (96%)	10 (4%)	0	100	100
1	D	245/288 (85%)	239 (98%)	5 (2%)	1 (0%)	38	25
All	All	988/1152 (86%)	953 (96%)	33 (3%)	2 (0%)	51	41

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	208	LEU
1	D	208	LEU

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	206/231 (89%)	203 (98%)	3 (2%)	70	65
1	B	199/231 (86%)	196 (98%)	3 (2%)	70	65
1	C	200/231 (87%)	199 (100%)	1 (0%)	91	90
1	D	199/231 (86%)	197 (99%)	2 (1%)	80	78
All	All	804/924 (87%)	795 (99%)	9 (1%)	78	75

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	141	ARG
1	A	166	GLN
1	B	2	GLU
1	B	43	SER
1	B	152	SER
1	C	211	VAL
1	D	2	GLU
1	D	216	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	140	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

9 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	NAP	A	1269	-	44,52,52	0.90	1 (2%)	51,80,80	1.75	6 (11%)
3	UEN	A	1270	-	26,27,27	2.72	11 (42%)	29,38,38	2.73	11 (37%)
4	ACT	A	1271	-	1,3,3	1.95	0	0,3,3	0.00	-
2	NAP	B	1269	-	44,52,52	1.12	3 (6%)	51,80,80	1.54	6 (11%)
3	UEN	B	1270	-	26,27,27	2.67	11 (42%)	29,38,38	2.52	12 (41%)
2	NAP	C	1269	-	44,52,52	1.00	1 (2%)	51,80,80	1.53	8 (15%)
3	UEN	C	1270	-	26,27,27	2.61	11 (42%)	29,38,38	2.67	11 (37%)
2	NAP	D	1269	-	44,52,52	1.05	3 (6%)	51,80,80	1.40	7 (13%)
3	UEN	D	1270	-	26,27,27	2.51	11 (42%)	29,38,38	2.77	11 (37%)

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	NAP	A	1269	-	-	0/27/67/67	0/5/5/5
3	UEN	A	1270	-	-	0/8/16/16	0/4/4/4
4	ACT	A	1271	-	-	0/0/0/0	0/0/0/0
2	NAP	B	1269	-	-	0/27/67/67	0/5/5/5
3	UEN	B	1270	-	-	0/8/16/16	0/4/4/4
2	NAP	C	1269	-	-	0/27/67/67	0/5/5/5
3	UEN	C	1270	-	-	0/8/16/16	0/4/4/4
2	NAP	D	1269	-	-	0/27/67/67	0/5/5/5
3	UEN	D	1270	-	-	0/8/16/16	0/4/4/4

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1270	UEN	CAT-C5	-6.21	1.30	1.41
3	B	1270	UEN	CAT-C5	-5.33	1.31	1.41
3	C	1270	UEN	CAT-C5	-5.27	1.31	1.41
3	C	1270	UEN	CAC-CAQ	-4.67	1.27	1.37
3	D	1270	UEN	CAT-C5	-4.35	1.33	1.41
3	D	1270	UEN	CAD-CAQ	-3.91	1.29	1.37
3	D	1270	UEN	CAC-CAQ	-3.62	1.29	1.37
3	A	1270	UEN	CAD-CAQ	-3.46	1.30	1.37
3	C	1270	UEN	C5-C4	-3.08	1.34	1.43
3	A	1270	UEN	C5-C4	-3.06	1.34	1.43
3	B	1270	UEN	CAC-CAQ	-3.00	1.31	1.37
3	D	1270	UEN	C5-C4	-2.98	1.35	1.43
3	B	1270	UEN	C5-C4	-2.90	1.35	1.43
3	A	1270	UEN	CAC-CAQ	-2.88	1.31	1.37
3	B	1270	UEN	C4-N3	-2.35	1.32	1.36
3	A	1270	UEN	C6-C5	-2.20	1.41	1.44
3	C	1270	UEN	CAD-CAQ	-2.11	1.32	1.37
3	A	1270	UEN	CAT-CAS	2.01	1.53	1.49
2	D	1269	NAP	C5A-C4A	2.01	1.45	1.40
3	D	1270	UEN	C2-NAA	2.19	1.38	1.34
3	A	1270	UEN	CAC-CAE	2.23	1.42	1.38
3	D	1270	UEN	C4-NAP	2.27	1.39	1.34
3	C	1270	UEN	C4-NAP	2.30	1.39	1.34
3	D	1270	UEN	CAT-CAS	2.30	1.53	1.49
3	C	1270	UEN	C2-NAA	2.31	1.38	1.34
3	B	1270	UEN	C4-NAP	2.31	1.39	1.34
2	D	1269	NAP	C2A-N3A	2.34	1.36	1.32
2	B	1269	NAP	C5N-C4N	2.41	1.43	1.38
3	B	1270	UEN	C6-N1	2.42	1.36	1.33
3	C	1270	UEN	CAT-CAS	2.45	1.53	1.49
3	D	1270	UEN	CAF-CAS	2.50	1.44	1.39
2	B	1269	NAP	C5A-C4A	2.70	1.46	1.40
2	C	1269	NAP	P2B-O2B	3.04	1.64	1.59
2	A	1269	NAP	P2B-O2B	3.08	1.65	1.59
3	B	1270	UEN	CAG-NAP	3.27	1.43	1.36
2	D	1269	NAP	P2B-O2B	3.32	1.65	1.59
3	B	1270	UEN	C2-NAA	3.44	1.41	1.34
3	A	1270	UEN	CAF-CAS	3.49	1.46	1.39
3	C	1270	UEN	CAE-CAS	3.49	1.46	1.39
3	C	1270	UEN	CAG-NAP	3.61	1.44	1.36
2	B	1269	NAP	P2B-O2B	3.62	1.65	1.59
3	D	1270	UEN	CAG-NAP	3.75	1.44	1.36
3	B	1270	UEN	CAE-CAS	4.25	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1270	UEN	CAG-NAP	4.39	1.45	1.36
3	C	1270	UEN	CAF-CAS	4.41	1.48	1.39
3	D	1270	UEN	CAE-CAS	4.57	1.49	1.39
3	A	1270	UEN	CAE-CAS	4.97	1.49	1.39
3	B	1270	UEN	CAF-CAS	5.28	1.50	1.39
3	B	1270	UEN	C6-NAO	5.93	1.45	1.35
3	C	1270	UEN	C6-NAO	6.55	1.46	1.35
3	D	1270	UEN	C6-NAO	6.61	1.46	1.35
3	A	1270	UEN	C6-NAO	6.68	1.46	1.35

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1269	NAP	N3A-C2A-N1A	-9.33	120.73	128.86
2	B	1269	NAP	N3A-C2A-N1A	-5.87	123.74	128.86
3	C	1270	UEN	N3-C2-N1	-5.43	119.53	127.46
2	C	1269	NAP	N3A-C2A-N1A	-5.35	124.20	128.86
3	B	1270	UEN	N3-C2-N1	-5.19	119.89	127.46
3	D	1270	UEN	N3-C2-N1	-5.09	120.03	127.46
3	D	1270	UEN	CAF-CAS-CAE	-4.79	108.08	117.59
3	A	1270	UEN	CAF-CAS-CAE	-4.52	108.61	117.59
2	C	1269	NAP	C4B-O4B-C1B	-4.12	105.38	109.77
3	A	1270	UEN	N3-C2-N1	-3.96	121.68	127.46
2	D	1269	NAP	N3A-C2A-N1A	-3.96	125.41	128.86
2	D	1269	NAP	C4B-O4B-C1B	-3.88	105.64	109.77
2	A	1269	NAP	C1B-N9A-C4A	-3.81	120.05	126.64
3	C	1270	UEN	CAF-CAS-CAE	-3.80	110.04	117.59
2	C	1269	NAP	C4D-O4D-C1D	-3.39	106.16	109.77
2	C	1269	NAP	C1B-N9A-C4A	-3.24	121.04	126.64
3	B	1270	UEN	CAF-CAS-CAE	-3.12	111.39	117.59
2	B	1269	NAP	C4B-O4B-C1B	-2.99	106.59	109.77
3	B	1270	UEN	CAK-CAX-NAO	-2.97	105.45	110.55
2	D	1269	NAP	C1B-N9A-C4A	-2.92	121.60	126.64
3	A	1270	UEN	CAI-CAK-CAX	-2.52	107.41	111.11
2	D	1269	NAP	C4A-C5A-N7A	-2.50	106.99	109.41
2	B	1269	NAP	C1B-N9A-C4A	-2.39	122.51	126.64
2	C	1269	NAP	C4A-C5A-N7A	-2.25	107.24	109.41
2	A	1269	NAP	O4B-C4B-C3B	-2.17	100.86	105.17
3	C	1270	UEN	CAL-CAX-CAK	-2.14	107.40	110.85
3	B	1270	UEN	CAL-CAX-CAK	-2.11	107.45	110.85
3	D	1270	UEN	C5-C6-N1	-2.06	118.56	122.15
2	C	1269	NAP	O2N-PN-O1N	2.03	122.78	112.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1269	NAP	C3N-C7N-N7N	2.04	120.11	117.77
2	A	1269	NAP	O3X-P2B-O2X	2.05	115.87	107.61
3	B	1270	UEN	CAF-CAD-CAQ	2.07	120.53	118.35
2	A	1269	NAP	O2N-PN-O1N	2.08	123.04	112.28
3	C	1270	UEN	CAE-CAC-CAQ	2.18	120.64	118.35
3	A	1270	UEN	CAE-CAS-CAT	2.23	124.65	120.86
3	D	1270	UEN	CAE-CAS-CAT	2.32	124.81	120.86
3	B	1270	UEN	C2-N1-C6	2.35	119.79	114.51
3	C	1270	UEN	NAA-C2-N1	2.35	121.00	117.24
3	D	1270	UEN	CAE-CAC-CAQ	2.36	120.83	118.35
2	B	1269	NAP	O2A-PA-O1A	2.42	124.81	112.28
3	A	1270	UEN	NAA-C2-N1	2.45	121.16	117.24
2	D	1269	NAP	C2A-N1A-C6A	2.49	123.12	118.77
2	C	1269	NAP	O3X-P2B-O2X	2.55	117.89	107.61
2	B	1269	NAP	C3N-C7N-N7N	2.58	120.72	117.77
2	A	1269	NAP	C3N-C7N-N7N	2.59	120.73	117.77
2	D	1269	NAP	O3X-P2B-O2X	2.71	118.56	107.61
3	D	1270	UEN	C2-N3-C4	2.95	118.61	115.16
3	B	1270	UEN	CAE-CAC-CAQ	2.96	121.46	118.35
3	A	1270	UEN	C2-N1-C6	3.03	121.33	114.51
2	D	1269	NAP	C3N-C7N-N7N	3.05	121.26	117.77
3	B	1270	UEN	CAE-CAS-CAT	3.08	126.10	120.86
3	A	1270	UEN	CAF-CAS-CAT	3.17	126.25	120.86
3	C	1270	UEN	CAF-CAS-CAT	3.23	126.36	120.86
3	B	1270	UEN	NAA-C2-N1	3.23	122.40	117.24
3	C	1270	UEN	CAF-CAD-CAQ	3.30	121.82	118.35
3	C	1270	UEN	C2-N1-C6	3.32	122.00	114.51
3	A	1270	UEN	C5-C6-NAO	3.34	124.10	120.61
3	D	1270	UEN	CAF-CAS-CAT	3.36	126.57	120.86
2	B	1269	NAP	O3X-P2B-O2X	3.42	121.42	107.61
3	D	1270	UEN	C2-N1-C6	3.46	122.30	114.51
3	C	1270	UEN	C2-N3-C4	3.55	119.31	115.16
3	A	1270	UEN	CAE-CAC-CAQ	3.66	122.20	118.35
3	D	1270	UEN	CAF-CAD-CAQ	3.88	122.43	118.35
3	A	1270	UEN	CAF-CAD-CAQ	4.85	123.46	118.35
3	B	1270	UEN	C2-N3-C4	4.92	120.90	115.16
3	B	1270	UEN	C5-C6-NAO	4.98	125.81	120.61
3	D	1270	UEN	C5-C6-NAO	5.49	126.34	120.61
3	B	1270	UEN	CAT-C5-C4	5.57	111.98	107.54
3	C	1270	UEN	C5-C6-NAO	5.81	126.67	120.61
3	C	1270	UEN	CAT-C5-C4	6.61	112.81	107.54
3	D	1270	UEN	CAT-C5-C4	7.80	113.76	107.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1270	UEN	CAT-C5-C4	8.41	114.25	107.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1269	NAP	1	0
3	A	1270	UEN	1	0
4	A	1271	ACT	1	0
3	B	1270	UEN	2	0
2	C	1269	NAP	1	0
2	D	1269	NAP	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	251/288 (87%)	-0.00	11 (4%) 35 45	9, 15, 34, 56	0
1	B	250/288 (86%)	-0.08	7 (2%) 53 64	9, 15, 31, 54	0
1	C	249/288 (86%)	0.01	10 (4%) 39 49	9, 15, 36, 62	0
1	D	249/288 (86%)	0.03	8 (3%) 48 59	8, 16, 35, 55	0
All	All	999/1152 (86%)	-0.01	36 (3%) 43 54	8, 15, 35, 62	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	113	GLY	8.0
1	B	113	GLY	4.8
1	C	212	ALA	4.7
1	D	211	VAL	4.4
1	A	151	SER	4.2
1	B	152	SER	4.1
1	D	221	TRP	3.8
1	C	152	SER	3.8
1	A	2	GLU	3.7
1	B	104	GLN	3.6
1	A	104	GLN	3.4
1	A	113	GLY	3.2
1	A	212	ALA	3.1
1	C	221	TRP	3.0
1	C	211	VAL	2.9
1	D	2	GLU	2.8
1	B	221	TRP	2.8
1	A	219	ASP	2.8
1	C	223	ARG	2.7
1	C	2	GLU	2.7
1	C	256	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	211	VAL	2.6
1	D	268	ALA	2.6
1	D	219	ASP	2.6
1	B	2	GLU	2.4
1	B	256	ILE	2.4
1	C	216	GLU	2.4
1	A	211	VAL	2.3
1	C	202	VAL	2.3
1	A	223	ARG	2.3
1	A	221	TRP	2.3
1	D	256	ILE	2.3
1	D	223	ARG	2.2
1	A	216	GLU	2.0
1	A	53[A]	SER	2.0
1	D	257	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
3	UEN	C	1270	24/24	0.91	0.12	0.43	13,18,34,44	0
3	UEN	B	1270	24/24	0.93	0.10	-0.01	11,16,26,33	0
3	UEN	D	1270	24/24	0.92	0.12	-0.11	14,19,33,44	0
3	UEN	A	1270	24/24	0.94	0.09	-0.39	14,19,26,33	0
2	NAP	B	1269	48/48	0.97	0.08	-0.75	9,12,16,19	0
4	ACT	A	1271	4/4	0.98	0.08	-0.84	15,15,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NAP	D	1269	48/48	0.98	0.07	-0.90	10,13,16,17	0
2	NAP	A	1269	48/48	0.98	0.07	-0.91	8,12,15,15	0
2	NAP	C	1269	48/48	0.98	0.07	-1.29	10,12,13,14	0

6.5 Other polymers [i](#)

There are no such residues in this entry.