



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:55 AM GMT

PDB ID : 3NKR  
Title : Crystal structure of mouse autotaxin in complex with 22:6-LPA  
Authors : Nishimasu, H.; Ishitani, R.; Mihara, E.; Takagi, J.; Aoki, J.; Nureki, O.  
Deposited on : 2010-06-20  
Resolution : 1.70 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

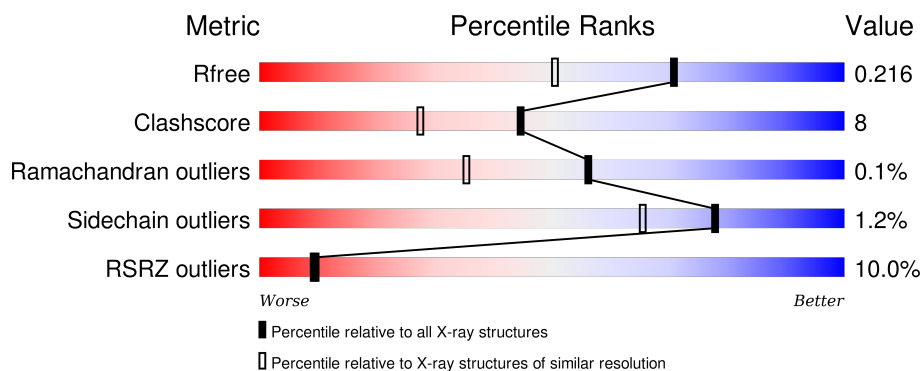
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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  $\geq 3$ , 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	831	<div> <div>9%</div> <div>81%</div> <div>13%</div> <div>6%</div> </div>

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
10	EDO	A	1012	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	EDO	A	1014	-	-	-	X
10	EDO	A	1015	-	-	-	X
10	EDO	A	1020	-	-	-	X
10	EDO	A	1021	-	-	-	X
10	EDO	A	1024	-	-	X	X
3	MAN	A	904	-	-	-	X
8	NKR	A	1007	-	-	-	X
9	SCN	A	1008	-	-	-	X

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 7130 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 Ectonucleotide pyrophosphatase/phosphodiesterase family member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	779	Total	C	N	O	S	0	5	0
			6234	3964	1062	1158	50			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LYS	SEE REMARK 999	UNP Q9R1E6
A	?	-	VAL	SEE REMARK 999	UNP Q9R1E6
A	?	-	GLU	SEE REMARK 999	UNP Q9R1E6
A	?	-	PRO	SEE REMARK 999	UNP Q9R1E6
A	859	SER	-	EXPRESSION TAG	UNP Q9R1E6
A	860	ARG	-	EXPRESSION TAG	UNP Q9R1E6
A	861	GLU	-	EXPRESSION TAG	UNP Q9R1E6
A	862	ASN	-	EXPRESSION TAG	UNP Q9R1E6
A	863	LEU	-	EXPRESSION TAG	UNP Q9R1E6
A	864	TYR	-	EXPRESSION TAG	UNP Q9R1E6
A	865	PHE	-	EXPRESSION TAG	UNP Q9R1E6
A	866	GLN	-	EXPRESSION TAG	UNP Q9R1E6

- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total	C	N	O	0	0
			28	16	2	10		
2	A	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Zn	0	0
			2	2		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		

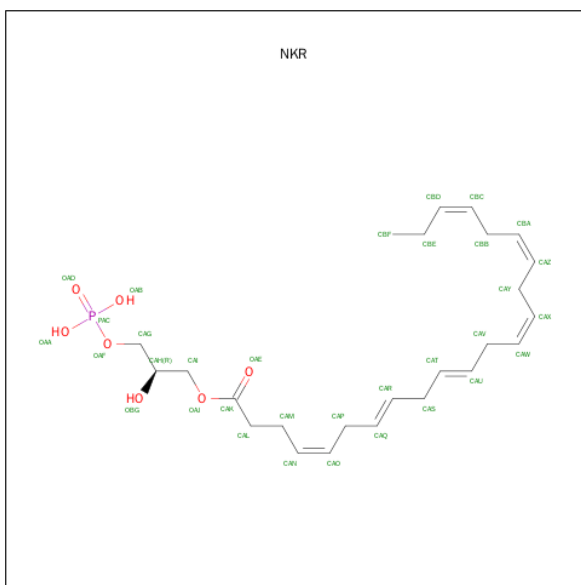
- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Na	0	0
			1	1		

- Molecule 7 is POTASSIUM ION (three-letter code: K) (formula: K).

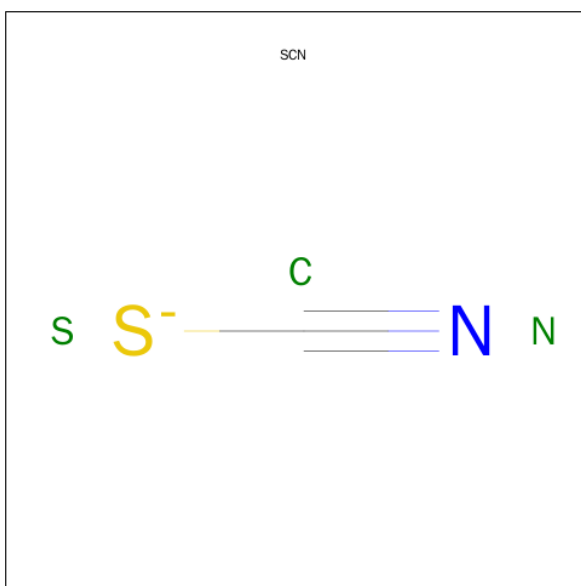
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	K	0	0
			1	1		

- Molecule 8 is (2R)-2-HYDROXY-3-(PHOSPHONOXY)PROPYL (4Z,7E,10E,13Z,16Z,19Z)-DOCOSA-4,7,10,13,16,19-HEXAENOATE (three-letter code: NKR) (formula: C<sub>25</sub>H<sub>39</sub>O<sub>7</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
8	A	1	Total	C	O	P	0	0	
			33	25	7	1			
8	A	1	Total	C				0	0
			18	18					

- Molecule 9 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total 3	C 1	N 1	S 1	0	0
9	A	1	Total 3	C 1	N 1	S 1	0	0

- Molecule 10 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

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

- Molecule 11 is water.

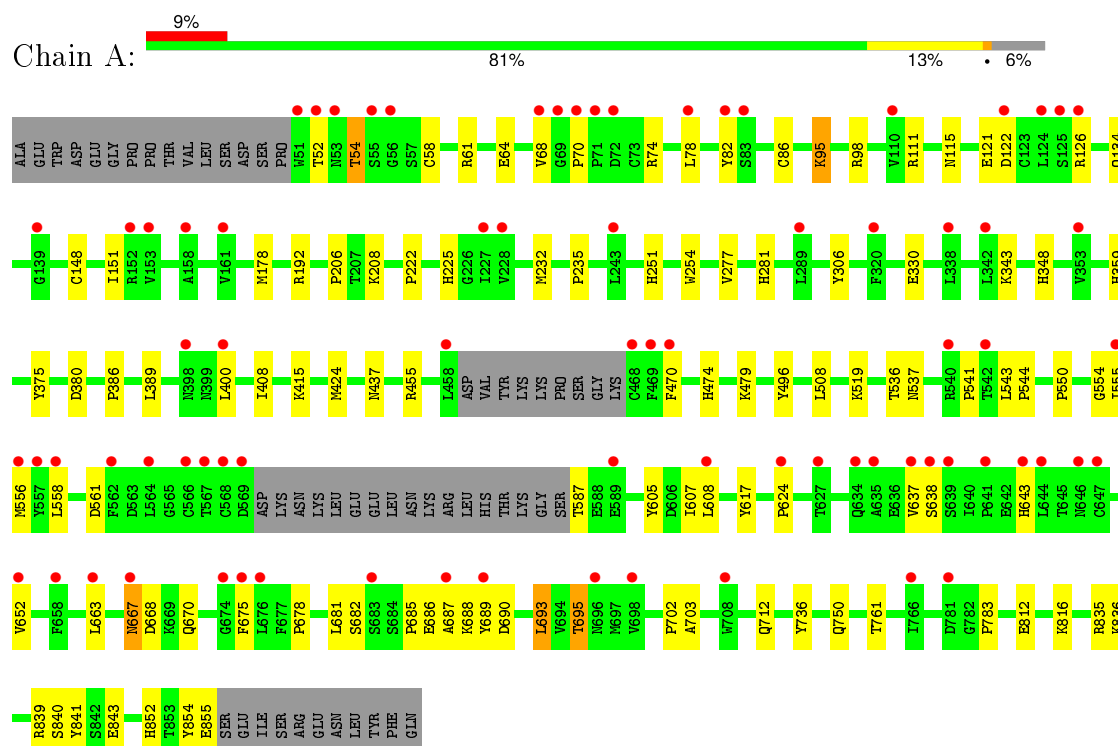
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	622	Total 622	O 622	0	0



### 3 Residue-property plots

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

- Molecule 1: Ectonucleotide pyrophosphatase/phosphodiesterase family member 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.54Å 94.11Å 75.31Å 90.00° 95.26° 90.00°	Depositor
Resolution (Å)	24.89 – 1.70 24.89 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.1 (24.89-1.70) 99.1 (24.89-1.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.30 (at 1.71Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6 _289)	Depositor
R, $R_{free}$	0.192 , 0.220 0.191 , 0.216	Depositor DCC
$R_{free}$ test set	4625 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.9	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 53.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 92307 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7130	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, BMA, NAG, NA, K, EDO, NKR, SCN, CA, MAN

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	0.43	0/6430	0.59	0/8746

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6234	0	5915	96	1
2	A	56	0	50	0	0
3	A	72	0	61	2	0
4	A	2	0	0	0	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
7	A	1	0	0	0	0
8	A	51	0	62	10	0
9	A	6	0	0	1	0
10	A	84	0	126	19	0
11	A	622	0	0	14	2
All	All	7130	0	6214	101	2

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 8.

All (101) 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)
3:A:904:MAN:O4	8:A:1007:NKR:HAP	1.49	1.10
1:A:208:LYS:HG3	9:A:1008:SCN:S	2.10	0.91
3:A:904:MAN:O4	8:A:1007:NKR:CAP	2.22	0.87
1:A:134:GLN:NE2	11:A:1484:HOH:O	2.06	0.86
1:A:835:ARG:HH21	10:A:1024:EDO:H11	1.42	0.84
1:A:254:TRP:O	8:A:1007:NKR:HASA	1.77	0.83
1:A:78:LEU:O	1:A:82:TYR:HD1	1.65	0.79
1:A:852:HIS:HD2	1:A:854:TYR:CZ	2.03	0.76
1:A:235:PRO:HG2	11:A:1226:HOH:O	1.88	0.73
1:A:251:HIS:O	8:A:1007:NKR:HAS	1.90	0.71
1:A:836:LYS:HE2	10:A:1024:EDO:H21	1.74	0.69
1:A:835:ARG:HE	10:A:1024:EDO:C2	2.07	0.68
1:A:389:LEU:CD1	11:A:1470:HOH:O	2.42	0.67
1:A:840:SER:OG	1:A:843:GLU:HG3	1.95	0.66
1:A:682:SER:OG	1:A:688:LYS:NZ	2.28	0.66
1:A:330:GLU:HG2	11:A:1483:HOH:O	1.96	0.65
1:A:675:PHE:H	10:A:1012:EDO:H11	1.61	0.64
1:A:254:TRP:O	8:A:1007:NKR:CAS	2.47	0.63
8:A:1006:NKR:CAU	8:A:1006:NKR:HAZ	2.28	0.63
1:A:68:VAL:O	1:A:74:ARG:HD2	1.99	0.62
1:A:78:LEU:O	1:A:82:TYR:CD1	2.48	0.62
1:A:281:HIS:ND1	10:A:1023:EDO:H21	2.15	0.62
1:A:835:ARG:HE	10:A:1024:EDO:H22	1.64	0.62
1:A:98:ARG:HG3	1:A:115:ASN:OD1	2.00	0.61
1:A:555:ILE:HG12	1:A:652:VAL:HG23	1.83	0.60
1:A:519:LYS:HE3	11:A:1206:HOH:O	2.01	0.60
1:A:702:PRO:HB2	10:A:1025:EDO:H22	1.84	0.60
1:A:678:PRO:HB3	1:A:712:GLN:HB3	1.83	0.59
1:A:122:ASP:HA	11:A:1467:HOH:O	2.04	0.58
1:A:121:GLU:O	11:A:1467:HOH:O	2.17	0.57
1:A:558:LEU:N	1:A:561:ASP:OD2	2.28	0.57
1:A:61:ARG:HD2	1:A:64:GLU:OE1	2.04	0.56
8:A:1006:NKR:CAZ	8:A:1006:NKR:CAT	2.83	0.56
1:A:408:ILE:HD11	1:A:424:MET:SD	2.45	0.56
1:A:617:TYR:CE1	1:A:695:THR:HG22	2.41	0.56
1:A:254:TRP:O	8:A:1007:NKR:HAU	2.05	0.56
1:A:675:PHE:H	10:A:1012:EDO:C1	2.18	0.55
1:A:558:LEU:O	1:A:561:ASP:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:VAL:HG22	11:A:1404:HOH:O	2.06	0.55
1:A:685:PRO:O	1:A:689:TYR:HD2	1.90	0.54
1:A:222:PRO:HA	1:A:225:HIS:CE1	2.42	0.54
1:A:389:LEU:HD12	11:A:1470:HOH:O	2.03	0.54
1:A:587:THR:N	11:A:1368:HOH:O	2.40	0.53
1:A:835:ARG:NH2	10:A:1024:EDO:H11	2.19	0.53
8:A:1006:NKR:HAZ	8:A:1006:NKR:CAT	2.39	0.53
1:A:151:ILE:HD12	10:A:1011:EDO:H21	1.91	0.53
1:A:111:ARG:NH2	1:A:126:ARG:HD3	2.24	0.52
1:A:678:PRO:HG2	1:A:681:LEU:HD12	1.93	0.51
1:A:306:TYR:CD2	8:A:1006:NKR:HAPA	2.47	0.50
1:A:550:PRO:HB3	1:A:605:TYR:CE1	2.46	0.50
1:A:348:HIS:CD2	1:A:348:HIS:H	2.30	0.50
1:A:687:ALA:O	1:A:690:ASP:HB2	2.12	0.50
1:A:343:LYS:HA	1:A:348:HIS:CD2	2.48	0.49
1:A:678:PRO:CG	1:A:681:LEU:HD12	2.42	0.49
1:A:663:LEU:O	1:A:667:ASN:HB3	2.12	0.49
1:A:281:HIS:ND1	10:A:1023:EDO:C2	2.76	0.49
1:A:690:ASP:O	1:A:693:LEU:HB2	2.12	0.49
1:A:206:PRO:HB3	1:A:389:LEU:HD13	1.94	0.49
1:A:178:MET:HE2	1:A:192:ARG:HD3	1.95	0.48
1:A:536:THR:O	1:A:537:ASN:HB2	2.14	0.48
1:A:359:HIS:CE1	1:A:474:HIS:CE1	3.02	0.48
1:A:554:GLY:O	1:A:556:MET:SD	2.72	0.48
1:A:64:GLU:OE2	11:A:1475:HOH:O	2.20	0.47
1:A:638:SER:OG	1:A:688:LYS:NZ	2.41	0.47
1:A:437:ASN:HD21	10:A:1030:EDO:C2	2.27	0.47
1:A:437:ASN:HD21	10:A:1030:EDO:H22	1.80	0.47
1:A:543:LEU:HD12	1:A:544:PRO:HD2	1.97	0.47
1:A:555:ILE:HG12	1:A:652:VAL:CG2	2.45	0.47
1:A:839:ARG:HE	10:A:1026:EDO:C2	2.28	0.47
1:A:95:LYS:NZ	11:A:1171:HOH:O	2.47	0.46
1:A:835:ARG:HB3	10:A:1024:EDO:H22	1.98	0.46
1:A:415:LYS:HE2	1:A:415:LYS:HB3	1.60	0.46
1:A:380:ASP:HA	1:A:455:ARG:NH1	2.31	0.45
1:A:637:VAL:HG22	1:A:681:LEU:HD23	1.99	0.45
1:A:148[B]:CYS:SG	1:A:496:TYR:HE2	2.39	0.45
1:A:637:VAL:HG22	1:A:681:LEU:CD2	2.47	0.44
1:A:95:LYS:HG3	11:A:1053:HOH:O	2.17	0.44
1:A:178:MET:HE2	1:A:178:MET:HB3	1.79	0.44
1:A:52:THR:OG1	1:A:70:PRO:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:761:THR:HA	10:A:1015:EDO:H12	2.00	0.44
1:A:617:TYR:HA	1:A:624:PRO:HA	2.00	0.44
1:A:667:ASN:ND2	1:A:667:ASN:C	2.71	0.43
1:A:667:ASN:ND2	1:A:668:ASP:N	2.66	0.43
1:A:670:GLN:NE2	11:A:1424:HOH:O	2.51	0.43
1:A:852:HIS:HD2	1:A:854:TYR:CE1	2.36	0.43
1:A:736:TYR:OH	1:A:750:GLN:HB3	2.18	0.43
1:A:479:LYS:O	1:A:855:GLU:HG3	2.19	0.43
1:A:54:THR:OG1	1:A:54:THR:O	2.34	0.43
1:A:703:ALA:N	10:A:1025:EDO:H21	2.34	0.42
1:A:783:PRO:HA	10:A:1026:EDO:H21	2.01	0.42
1:A:375:TYR:OH	1:A:415:LYS:HD3	2.19	0.42
1:A:58:CYS:SG	1:A:86:CYS:HB2	2.60	0.42
1:A:550:PRO:HB2	1:A:607:ILE:HG12	2.03	0.41
1:A:667:ASN:HD22	1:A:668:ASP:N	2.18	0.41
1:A:643:HIS:CD2	1:A:643:HIS:H	2.38	0.41
1:A:835:ARG:NE	10:A:1024:EDO:H22	2.32	0.41
1:A:812:GLU:O	1:A:816:LYS:HG3	2.21	0.41
1:A:470:PHE:C	1:A:470:PHE:CD1	2.94	0.41
1:A:508:LEU:HD23	1:A:508:LEU:HA	1.93	0.40
1:A:389:LEU:HD23	1:A:389:LEU:N	2.37	0.40
1:A:541:PRO:HB2	1:A:841:TYR:CE2	2.57	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:927:HOH:O	11:A:1411:HOH:O[1_655]	2.01	0.19
1:A:400:LEU:O	11:A:1384:HOH:O[2_655]	2.19	0.01

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	778/831 (94%)	758 (97%)	19 (2%)	1 (0%)	56 35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	386	PRO

### 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	693/756 (92%)	685 (99%)	8 (1%)	78 65

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	THR
1	A	95	LYS
1	A	232	MET
1	A	608	LEU
1	A	667	ASN
1	A	686	GLU
1	A	693	LEU
1	A	695	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	GLN
1	A	326	ASN
1	A	337	GLN
1	A	348	HIS
1	A	374	ASN
1	A	643	HIS
1	A	667	ASN

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Mol	Chain	Res	Type
1	A	802	ASN
1	A	827	HIS

### 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 ⓘ

10 carbohydrates 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	NAG	A	898	1,2	14,14,15	0.66	0	15,19,21	1.30	1 (6%)
2	NAG	A	899	2	14,14,15	0.46	0	15,19,21	2.10	2 (13%)
3	NAG	A	900	1,3	14,14,15	0.42	0	15,19,21	0.83	0
3	NAG	A	901	3	14,14,15	0.53	0	15,19,21	0.96	0
3	BMA	A	902	3	11,11,12	0.77	0	14,15,17	1.31	2 (14%)
3	MAN	A	903	3	11,11,12	0.66	0	14,15,17	1.01	0
3	MAN	A	904	3	11,11,12	0.57	0	14,15,17	1.22	2 (14%)
3	MAN	A	905	3	11,11,12	0.68	0	14,15,17	0.92	0
2	NAG	A	907	1,2	14,14,15	0.64	0	15,19,21	0.96	0
2	NAG	A	908	2	14,14,15	0.62	0	15,19,21	1.20	2 (13%)

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	NAG	A	898	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	899	2	-	0/6/23/26	0/1/1/1
3	NAG	A	900	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	901	3	-	0/6/23/26	0/1/1/1
3	BMA	A	902	3	-	0/2/19/22	0/1/1/1
3	MAN	A	903	3	-	0/2/19/22	0/1/1/1
3	MAN	A	904	3	-	0/2/19/22	0/1/1/1
3	MAN	A	905	3	-	0/2/19/22	0/1/1/1
2	NAG	A	907	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	908	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	904	MAN	C2-C3-C4	-3.15	105.69	111.04
3	A	902	BMA	O5-C1-C2	-3.08	105.86	110.86
2	A	908	NAG	C3-C4-C5	-2.55	105.75	110.20
3	A	904	MAN	O5-C1-C2	-2.07	107.51	110.86
3	A	902	BMA	C3-C4-C5	2.06	113.79	110.20
2	A	899	NAG	C3-C4-C5	2.07	113.80	110.20
2	A	908	NAG	C1-O5-C5	2.54	115.48	112.25
2	A	898	NAG	C1-O5-C5	4.07	117.42	112.25
2	A	899	NAG	C1-O5-C5	7.11	121.28	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	904	MAN	2	0

## 5.6 Ligand geometry

Of 30 ligands modelled in this entry, 5 are monoatomic - leaving 25 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length

(or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
8	NKR	A	1006	4	32,32,32	1.55	5 (15%)	34,36,36	1.26	4 (11%)
8	NKR	A	1007	-	17,17,32	2.05	8 (47%)	16,16,36	1.50	2 (12%)
9	SCN	A	1008	-	2,2,2	1.65	1 (50%)	1,1,1	0.27	0
9	SCN	A	1009	-	2,2,2	1.88	1 (50%)	1,1,1	0.15	0
10	EDO	A	1010	-	3,3,3	0.48	0	2,2,2	0.57	0
10	EDO	A	1011	-	3,3,3	0.66	0	2,2,2	0.12	0
10	EDO	A	1012	-	3,3,3	0.39	0	2,2,2	0.66	0
10	EDO	A	1013	-	3,3,3	0.54	0	2,2,2	0.36	0
10	EDO	A	1014	-	3,3,3	0.55	0	2,2,2	0.21	0
10	EDO	A	1015	-	3,3,3	0.37	0	2,2,2	0.59	0
10	EDO	A	1016	-	3,3,3	0.52	0	2,2,2	0.22	0
10	EDO	A	1017	-	3,3,3	0.50	0	2,2,2	0.50	0
10	EDO	A	1018	-	3,3,3	0.60	0	2,2,2	0.32	0
10	EDO	A	1019	-	3,3,3	0.44	0	2,2,2	0.42	0
10	EDO	A	1020	-	3,3,3	0.46	0	2,2,2	0.43	0
10	EDO	A	1021	-	3,3,3	0.45	0	2,2,2	0.54	0
10	EDO	A	1022	-	3,3,3	0.51	0	2,2,2	0.40	0
10	EDO	A	1023	-	3,3,3	0.45	0	2,2,2	0.73	0
10	EDO	A	1024	-	3,3,3	0.51	0	2,2,2	0.31	0
10	EDO	A	1025	-	3,3,3	0.45	0	2,2,2	0.41	0
10	EDO	A	1026	-	3,3,3	0.35	0	2,2,2	0.48	0
10	EDO	A	1027	-	3,3,3	0.55	0	2,2,2	0.39	0
10	EDO	A	1028	-	3,3,3	0.54	0	2,2,2	0.39	0
10	EDO	A	1029	-	3,3,3	0.54	0	2,2,2	0.38	0
10	EDO	A	1030	-	3,3,3	0.47	0	2,2,2	0.13	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
8	NKR	A	1006	4	-	0/32/32/32	0/0/0/0
8	NKR	A	1007	-	-	0/15/15/32	0/0/0/0
9	SCN	A	1008	-	-	0/0/0/0	0/0/0/0
9	SCN	A	1009	-	-	0/0/0/0	0/0/0/0
10	EDO	A	1010	-	-	0/1/1/1	0/0/0/0
10	EDO	A	1011	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	EDO	A	1012	-	-	0/1/1/1	0/0/0/0
10	EDO	A	1013	-	-	0/1/1/1	0/0/0/0
10	EDO	A	1014	-	-	0/1/1/1	0/0/0/0
10	EDO	A	1015	-	-	0/1/1/1	0/0/0/0
10	EDO	A	1016	-	-	0/1/1/1	0/0/0/0
10	EDO	A	1017	-	-	0/1/1/1	0/0/0/0
10	EDO	A	1018	-	-	0/1/1/1	0/0/0/0
10	EDO	A	1019	-	-	0/1/1/1	0/0/0/0
10	EDO	A	1020	-	-	0/1/1/1	0/0/0/0
10	EDO	A	1021	-	-	0/1/1/1	0/0/0/0
10	EDO	A	1022	-	-	0/1/1/1	0/0/0/0
10	EDO	A	1023	-	-	0/1/1/1	0/0/0/0
10	EDO	A	1024	-	-	0/1/1/1	0/0/0/0
10	EDO	A	1025	-	-	0/1/1/1	0/0/0/0
10	EDO	A	1026	-	-	0/1/1/1	0/0/0/0
10	EDO	A	1027	-	-	0/1/1/1	0/0/0/0
10	EDO	A	1028	-	-	0/1/1/1	0/0/0/0
10	EDO	A	1029	-	-	0/1/1/1	0/0/0/0
10	EDO	A	1030	-	-	0/1/1/1	0/0/0/0

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1007	NKR	CAS-CAT	-3.10	1.34	1.51
8	A	1007	NKR	CBE-CBD	-2.80	1.37	1.51
8	A	1007	NKR	CAY-CAZ	-2.59	1.36	1.51
8	A	1007	NKR	CBB-CBC	-2.56	1.36	1.51
8	A	1007	NKR	CBB-CBA	-2.55	1.37	1.51
8	A	1006	NKR	CBE-CBD	-2.48	1.39	1.51
8	A	1007	NKR	CAP-CAQ	-2.44	1.39	1.51
8	A	1007	NKR	CAS-CAR	-2.41	1.37	1.51
8	A	1006	NKR	CAM-CAN	-2.36	1.39	1.50
8	A	1007	NKR	CAY-CAX	-2.28	1.38	1.51
8	A	1006	NKR	CAY-CAZ	-2.08	1.39	1.51
8	A	1006	NKR	CAS-CAT	-2.05	1.39	1.51
9	A	1008	SCN	C-S	2.32	1.78	1.63
9	A	1009	SCN	C-S	2.61	1.80	1.63
8	A	1006	NKR	PAC-OAB	2.65	1.64	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
8	A	1007	NKR	CBC-CBB-CBA	-4.58	96.75	112.00
8	A	1006	NKR	CAL-CAM-CAN	-3.26	104.70	112.79
8	A	1006	NKR	CAI-OAJ-CAK	-2.62	109.51	116.85
8	A	1006	NKR	OBG-CAH-CAG	-2.22	100.90	109.35
8	A	1007	NKR	CAW-CAV-CAU	-2.09	105.05	112.00
8	A	1006	NKR	OAA-PAC-OAF	2.26	113.08	106.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1006	NKR	4	0
8	A	1007	NKR	6	0
9	A	1008	SCN	1	0
10	A	1011	EDO	1	0
10	A	1012	EDO	2	0
10	A	1015	EDO	1	0
10	A	1023	EDO	2	0
10	A	1024	EDO	7	0
10	A	1025	EDO	2	0
10	A	1026	EDO	2	0
10	A	1030	EDO	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	779/831 (93%)	0.52	78 (10%) 9 9	13, 30, 54, 66	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	51	TRP	8.0
1	A	69	GLY	7.9
1	A	70	PRO	7.0
1	A	676	LEU	6.1
1	A	68	VAL	6.0
1	A	458	LEU	5.7
1	A	158	ALA	5.5
1	A	644	LEU	5.5
1	A	568	CYS	5.5
1	A	468	CYS	5.3
1	A	558	LEU	5.1
1	A	689	TYR	4.5
1	A	675	PHE	4.5
1	A	652	VAL	4.3
1	A	698	VAL	4.3
1	A	71	PRO	4.3
1	A	110	VAL	4.2
1	A	641	PRO	4.2
1	A	398	ASN	4.1
1	A	125[A]	SER	4.0
1	A	663	LEU	4.0
1	A	569	ASP	3.9
1	A	566	CYS	3.9
1	A	643	HIS	3.9
1	A	634	GLN	3.8
1	A	562	PHE	3.8
1	A	687	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	320	PHE	3.3
1	A	153	VAL	3.3
1	A	55	SER	3.3
1	A	161	VAL	3.2
1	A	589	GLU	3.1
1	A	564	LEU	3.1
1	A	52	THR	3.1
1	A	338	LEU	3.0
1	A	674	GLY	2.9
1	A	78	LEU	2.9
1	A	469	PHE	2.9
1	A	637	VAL	2.9
1	A	646	ASN	2.9
1	A	556	MET	2.8
1	A	152	ARG	2.8
1	A	766	ILE	2.8
1	A	243	LEU	2.8
1	A	353	VAL	2.7
1	A	72	ASP	2.6
1	A	624	PRO	2.6
1	A	781	ASP	2.6
1	A	555	ILE	2.6
1	A	139	GLY	2.6
1	A	56	GLY	2.5
1	A	683	SER	2.5
1	A	667	ASN	2.5
1	A	557	TYR	2.4
1	A	635	ALA	2.4
1	A	647	CYS	2.4
1	A	342	LEU	2.4
1	A	708	TRP	2.4
1	A	227	ILE	2.3
1	A	567	THR	2.3
1	A	696	ASN	2.3
1	A	289	LEU	2.3
1	A	608	LEU	2.2
1	A	627	THR	2.2
1	A	124	LEU	2.2
1	A	82	TYR	2.2
1	A	658	PHE	2.2
1	A	83	SER	2.2
1	A	228	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	126	ARG	2.1
1	A	122	ASP	2.1
1	A	53	ASN	2.1
1	A	540	ARG	2.1
1	A	400	LEU	2.1
1	A	639	SER	2.0
1	A	470	PHE	2.0
1	A	638	SER	2.0
1	A	542	THR	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	MAN	A	904	11/12	0.86	0.24	7.32	32,36,40,46	0
2	NAG	A	898	14/15	0.74	0.24	0.26	55,60,61,62	0
2	NAG	A	907	14/15	0.92	0.09	-0.05	25,30,38,43	0
3	NAG	A	900	14/15	0.97	0.09	-0.08	15,18,21,22	0
3	NAG	A	901	14/15	0.95	0.07	-	23,28,38,39	0
3	MAN	A	905	11/12	0.93	0.13	-	24,30,38,38	0
3	BMA	A	902	11/12	0.86	0.20	-	39,43,49,50	0
2	NAG	A	899	14/15	0.86	0.27	-	58,62,64,65	0
3	MAN	A	903	11/12	0.85	0.14	-	37,39,41,47	0
2	NAG	A	908	14/15	0.83	0.32	-	46,53,56,61	0

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
10	EDO	A	1021	4/4	0.93	0.18	5.87	31,37,38,45	0
9	SCN	A	1008	3/3	0.71	0.24	4.48	19,19,32,44	0
10	EDO	A	1015	4/4	0.90	0.16	4.23	27,28,33,36	0
8	NKR	A	1007	18/33	0.78	0.19	3.91	31,38,43,43	0
10	EDO	A	1012	4/4	0.90	0.31	3.72	33,36,38,41	0
10	EDO	A	1020	4/4	0.94	0.14	3.50	27,30,37,42	0
10	EDO	A	1024	4/4	0.89	0.18	3.26	39,40,43,47	0
10	EDO	A	1014	4/4	0.95	0.13	2.56	31,31,32,36	0
8	NKR	A	1006	33/33	0.94	0.15	1.56	19,36,41,46	0
10	EDO	A	1010	4/4	0.96	0.12	1.40	31,33,33,35	0
10	EDO	A	1011	4/4	0.83	0.15	1.11	27,28,34,36	0
10	EDO	A	1013	4/4	0.96	0.12	0.69	30,31,33,34	0
10	EDO	A	1028	4/4	0.98	0.08	0.55	22,23,23,24	0
9	SCN	A	1009	3/3	0.99	0.09	0.50	26,26,31,42	0
10	EDO	A	1029	4/4	0.93	0.10	0.40	27,29,29,34	0
10	EDO	A	1017	4/4	0.96	0.09	0.39	31,32,36,38	0
10	EDO	A	1030	4/4	0.97	0.10	0.20	19,30,33,37	0
10	EDO	A	1019	4/4	0.98	0.12	0.12	35,36,37,42	0
10	EDO	A	1023	4/4	0.95	0.10	0.11	28,29,32,35	0
10	EDO	A	1022	4/4	0.93	0.08	-0.21	37,38,40,45	0
7	K	A	1005	1/1	0.70	0.13	-0.46	44,44,44,44	0
10	EDO	A	1026	4/4	0.97	0.08	-0.79	26,32,36,38	0
10	EDO	A	1016	4/4	0.96	0.09	-0.88	28,31,31,33	0
5	CA	A	1003	1/1	0.99	0.05	-1.53	21,21,21,21	0
4	ZN	A	1002	1/1	1.00	0.05	-2.34	16,16,16,16	0
4	ZN	A	1001	1/1	1.00	0.05	-3.10	18,18,18,18	0
10	EDO	A	1027	4/4	0.87	0.17	-	33,34,40,40	0
10	EDO	A	1025	4/4	0.93	0.28	-	34,36,41,41	0
6	NA	A	1004	1/1	0.98	0.09	-	28,28,28,28	0
10	EDO	A	1018	4/4	0.92	0.12	-	25,30,35,36	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.