



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 12:08 AM GMT

PDB ID : 2VHW  
Title : CRYSTAL STRUCTURE OF HOLO L-ALANINE DEHYDROGENASE  
FROM MYCOBACTERIUM TUBERCULOSIS IN THE OPEN AND  
CLOSED CONFORMATION  
Authors : Agren, D.; Schneider, G.  
Deposited on : 2007-11-26  
Resolution : 2.00 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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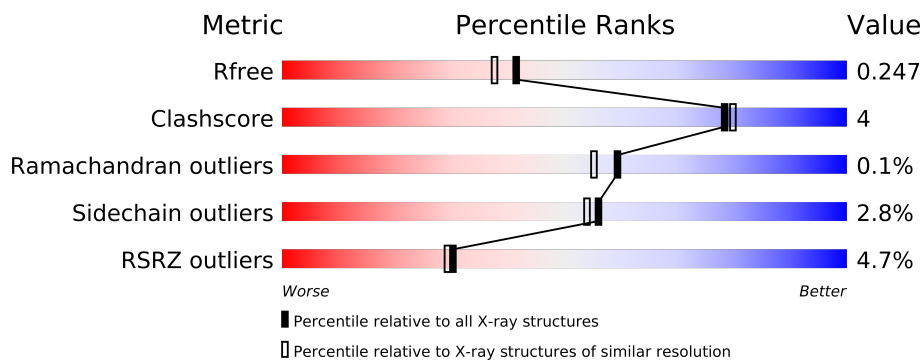
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.00 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))
$R_{free}$	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	377	
1	B	377	
1	C	377	
1	D	377	
1	E	377	
1	F	377	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18159 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

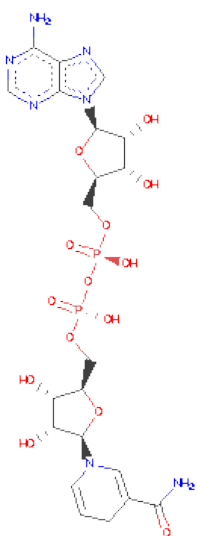
- Molecule 1 is a protein called ALANINE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	371	Total	C	N	O	S	0	0	0
			2719	1710	479	517	13			
1	B	370	Total	C	N	O	S	0	3	0
			2730	1717	479	521	13			
1	C	371	Total	C	N	O	S	0	0	0
			2719	1710	479	517	13			
1	D	370	Total	C	N	O	S	0	0	0
			2714	1707	478	516	13			
1	E	373	Total	C	N	O	S	0	1	0
			2747	1727	488	519	13			
1	F	373	Total	C	N	O	S	0	2	0
			2752	1730	488	521	13			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is 1,4-DIHYDRONICOTINAMIDEADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: C<sub>21</sub>H<sub>29</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



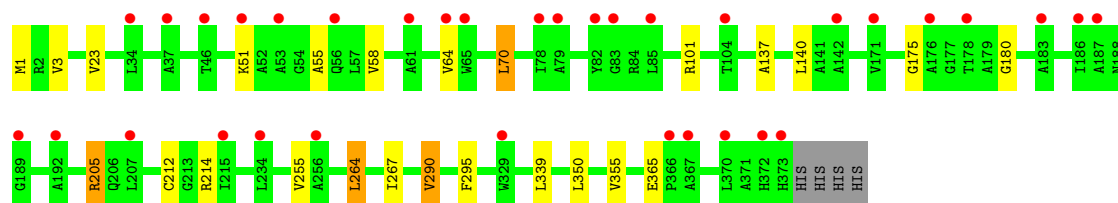
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is water.

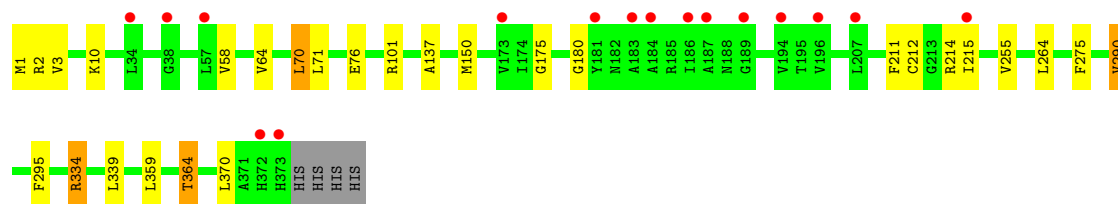
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	219	Total	O	0	0
			219	219		
4	B	310	Total	O	0	0
			310	310		
4	C	211	Total	O	0	0
			211	211		
4	D	297	Total	O	0	0
			297	297		
4	E	195	Total	O	0	0
			195	195		
4	F	280	Total	O	0	0
			280	280		



## ● Molecule 1: ALANINE DEHYDROGENASE

Chain E: 

## ● Molecule 1: ALANINE DEHYDROGENASE

Chain F: 

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	177.03Å 172.01Å 98.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.00 49.56 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (40.00-2.00) 94.6 (49.56-2.00)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.29 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.176 , 0.212 0.219 , 0.247	Depositor DCC
$R_{free}$ test set	9700 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.0	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 41.7	EDS
Estimated twinning fraction	0.014 for k,h,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 191725 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	18159	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, NAI

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	0.56	1/2769 (0.0%)	0.72	3/3773 (0.1%)
1	B	0.60	0/2789	0.76	4/3800 (0.1%)
1	C	0.53	0/2769	0.66	2/3773 (0.1%)
1	D	0.58	0/2764	0.67	1/3766 (0.0%)
1	E	0.52	0/2802	0.67	3/3817 (0.1%)
1	F	0.56	0/2810	0.68	1/3828 (0.0%)
All	All	0.56	1/16703 (0.0%)	0.69	14/22757 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	46	THR	CB-OG1	-5.76	1.31	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	272	GLY	N-CA-C	-10.27	87.42	113.10
1	B	272	GLY	N-CA-C	-8.68	91.39	113.10
1	E	205	ARG	NE-CZ-NH2	-8.31	116.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	272	GLY	N-CA-C	-7.83	93.51	113.10
1	E	205	ARG	NE-CZ-NH1	7.65	124.13	120.30
1	E	264	LEU	CA-CB-CG	7.35	132.21	115.30
1	F	334	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	B	71	LEU	CA-CB-CG	-6.25	100.92	115.30
1	D	214	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	B	294	LEU	CA-CB-CG	5.46	127.85	115.30
1	A	71	LEU	CA-CB-CG	-5.41	102.86	115.30
1	C	71	LEU	CA-CB-CG	-5.31	103.09	115.30
1	A	46	THR	OG1-CB-CG2	5.11	121.76	110.00
1	B	86	ARG	NE-CZ-NH1	-5.06	117.77	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	271	GLN	Peptide
1	B	271	GLN	Peptide
1	C	271	GLN	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2719	0	2732	21	0
1	B	2730	0	2743	14	0
1	C	2719	0	2732	32	0
1	D	2714	0	2727	23	0
1	E	2747	0	2759	19	0
1	F	2752	0	2763	20	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	44	0	27	1	0
3	B	44	0	27	1	0
3	C	44	0	27	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	44	0	27	3	0
3	E	44	0	27	2	0
3	F	44	0	27	1	0
4	A	219	0	0	0	0
4	B	310	0	0	1	0
4	C	211	0	0	1	0
4	D	297	0	0	3	0
4	E	195	0	0	3	0
4	F	280	0	0	3	0
All	All	18159	0	16618	120	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (120) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:101:ARG:HG3	1:C:101:ARG:HH21	1.18	1.04
1:C:241:VAL:HG23	1:C:244:ALA:HB3	1.57	0.87
1:C:101:ARG:CG	1:C:101:ARG:HH21	1.87	0.86
1:D:282:THR:HG22	1:D:284:ASP:H	1.43	0.83
1:B:255:VAL:HG11	1:B:290:VAL:HG22	1.63	0.78
1:C:329:TRP:HH2	1:C:369:VAL:HG12	1.49	0.76
1:D:214:ARG:NH2	1:F:212:CYS:O	2.20	0.72
1:C:101:ARG:NH2	1:C:101:ARG:HG3	1.96	0.71
1:D:241:VAL:HG23	1:D:244:ALA:HB3	1.72	0.70
1:C:329:TRP:HH2	1:C:369:VAL:CG1	2.05	0.70
1:C:361:VAL:HG22	1:C:362:PRO:HD2	1.72	0.70
1:D:318:MET:HG3	4:D:2126:HOH:O	1.92	0.69
1:D:353:GLU:O	1:D:357:THR:HG23	1.92	0.69
1:E:205:ARG:NH2	4:E:2104:HOH:O	2.26	0.68
1:F:334:ARG:HD2	1:F:370:LEU:O	1.95	0.67
1:E:350:LEU:HD21	1:E:355:VAL:HG12	1.78	0.66
1:C:75:LYS:NZ	4:C:2051:HOH:O	2.28	0.65
1:A:290:VAL:HG13	1:A:295:PHE:CD1	2.32	0.65
1:D:2:ARG:NH1	4:D:2002:HOH:O	2.29	0.64
1:B:296:TYR:CE2	1:B:298:VAL:HG13	2.32	0.64
1:C:214:ARG:HG3	1:E:214:ARG:HG3	1.81	0.63
1:E:255:VAL:HG11	1:E:290:VAL:HG22	1.79	0.62
1:C:31:HIS:HE1	1:C:326:ASP:OD1	1.85	0.60
1:D:290:VAL:HG13	1:D:295:PHE:CD1	2.37	0.59
1:C:241:VAL:CG2	1:C:244:ALA:HB3	2.32	0.59
1:A:255:VAL:HG11	1:A:290:VAL:HG22	1.84	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:365:GLU:HG3	4:D:2290:HOH:O	2.02	0.59
1:B:269:ILE:O	1:B:272:GLY:HA2	2.02	0.59
1:A:62:ASP:OD1	1:A:84:ARG:HD3	2.03	0.58
1:A:135:GLU:OE1	1:E:205:ARG:HD3	2.03	0.58
1:C:255:VAL:HG11	1:C:290:VAL:HG22	1.85	0.57
1:A:137:ALA:HB2	3:A:1373:NAI:H4N	1.86	0.57
1:F:255:VAL:HG11	1:F:290:VAL:HG22	1.85	0.56
1:C:101:ARG:NH2	1:C:101:ARG:CG	2.56	0.56
1:E:214:ARG:NH2	4:E:2116:HOH:O	2.23	0.56
1:C:1:MET:N	1:C:31:HIS:HD2	2.04	0.56
1:F:101[B]:ARG:NH2	1:F:359:LEU:O	2.37	0.56
1:B:214:ARG:NH2	4:B:2199:HOH:O	2.29	0.55
1:D:188:ASN:OD1	1:D:214:ARG:HD2	2.07	0.55
1:E:365:GLU:HG3	4:E:2192:HOH:O	2.07	0.55
1:D:264:LEU:HD13	1:D:293:THR:CG2	2.37	0.55
1:C:269:ILE:O	1:C:272:GLY:HA2	2.06	0.55
1:C:329:TRP:CH2	1:C:369:VAL:HG12	2.38	0.54
1:D:101:ARG:NH2	1:D:105:ASP:OD2	2.41	0.53
1:E:290:VAL:HG13	1:E:295:PHE:CD1	2.43	0.53
1:C:290:VAL:HG13	1:C:295:PHE:CD1	2.44	0.53
1:C:267:ILE:O	3:C:1372:NAI:H2N	2.09	0.52
1:F:137:ALA:HB2	3:F:1374:NAI:H4N	1.91	0.52
1:D:255:VAL:HG11	1:D:290:VAL:HG22	1.92	0.52
1:D:267:ILE:O	3:D:1371:NAI:H2N	2.10	0.52
1:F:290:VAL:HG13	1:F:295:PHE:CD1	2.45	0.51
1:B:137:ALA:HB2	3:B:1372:NAI:H4N	1.93	0.51
1:E:137:ALA:HB2	3:E:1374:NAI:H4N	1.93	0.51
1:F:10:LYS:HE3	1:F:76:GLU:OE2	2.10	0.51
1:D:264:LEU:HD13	1:D:293:THR:HG23	1.93	0.50
1:F:211:PHE:CD1	1:F:215:ILE:HD12	2.46	0.50
1:B:15:ARG:HD3	1:B:309:SER:HB3	1.94	0.50
1:A:306:PRO:HD2	1:C:157:GLY:HA3	1.94	0.49
1:F:214:ARG:NH2	4:F:2159:HOH:O	2.40	0.49
1:F:58:VAL:CG2	1:F:64:VAL:HG23	2.42	0.49
1:B:75:LYS:NZ	1:B:300:ASN:OD1	2.46	0.48
1:A:287:THR:HA	1:A:295:PHE:O	2.14	0.48
1:A:152:THR:HG21	1:C:283:TYR:CD2	2.48	0.48
1:A:346:HIS:CD2	1:A:369:VAL:HG21	2.48	0.48
1:B:2:ARG:HD3	1:B:67:ASP:O	2.14	0.48
1:A:7:THR:H	1:A:36:GLN:NE2	2.11	0.48
1:A:151:ARG:HD3	1:C:14:PHE:CD1	2.49	0.48
1:E:58:VAL:HG21	1:E:64:VAL:HG23	1.96	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:58:VAL:HG21	1:F:64:VAL:HG23	1.95	0.47
1:F:364:THR:CG2	4:F:2252:HOH:O	2.62	0.47
1:A:296:TYR:CE2	1:A:298:VAL:HG13	2.49	0.47
1:B:290:VAL:HG13	1:B:295:PHE:CD1	2.49	0.47
1:B:264:LEU:HB3	1:B:275:PHE:CE1	2.50	0.47
1:D:264:LEU:CD1	1:D:293:THR:HG23	2.45	0.47
1:F:364:THR:HG22	4:F:2252:HOH:O	2.14	0.46
1:B:287:THR:HA	1:B:295:PHE:O	2.14	0.46
1:D:15:ARG:HD3	1:D:309:SER:HB3	1.98	0.46
1:D:296:TYR:CE2	1:D:298:VAL:HG13	2.51	0.46
1:E:1:MET:SD	1:E:70:LEU:HB2	2.56	0.45
1:D:188:ASN:OD1	1:D:214:ARG:CD	2.64	0.45
1:E:58:VAL:CG2	1:E:64:VAL:HG23	2.47	0.45
1:C:279:ARG:HB2	1:C:280:PRO:HD2	1.98	0.45
1:A:331:ALA:HA	1:A:334:ARG:HD2	1.98	0.44
1:A:175:GLY:O	1:A:180:GLY:HA3	2.17	0.44
1:B:290:VAL:O	1:B:293:THR:HB	2.18	0.44
1:C:211:PHE:CD1	1:C:215:ILE:HD12	2.52	0.44
1:C:164:PRO:HG2	1:E:205:ARG:HG2	1.98	0.44
1:D:177:GLY:HA3	3:D:1371:NAI:O5B	2.18	0.44
1:F:58:VAL:HG21	1:F:64:VAL:CG2	2.48	0.44
1:C:365:GLU:O	1:C:368:SER:HB2	2.18	0.44
1:D:2:ARG:HD3	1:D:69:ASP:OD2	2.18	0.44
1:F:58:VAL:CG2	1:F:64:VAL:CG2	2.96	0.43
1:B:255:VAL:HG11	1:B:290:VAL:CG2	2.43	0.43
1:C:62:ASP:OD1	1:C:84:ARG:HD3	2.19	0.43
1:C:287:THR:HA	1:C:295:PHE:O	2.18	0.43
1:E:175:GLY:O	1:E:180:GLY:HA3	2.18	0.43
1:D:137:ALA:HB2	3:D:1371:NAI:H4N	2.01	0.42
1:E:23:VAL:HG11	1:E:55:ALA:HB2	2.00	0.42
1:A:205:ARG:HG2	1:B:164:PRO:HG2	2.01	0.42
1:A:269:ILE:O	1:A:272:GLY:HA2	2.19	0.42
1:A:346:HIS:HD2	1:A:369:VAL:HG21	1.83	0.42
1:A:75:LYS:HD2	1:A:75:LYS:HA	1.87	0.42
1:A:14:PHE:HB2	1:A:306:PRO:HG3	2.02	0.42
1:A:15:ARG:HD3	1:A:309:SER:HB3	2.02	0.42
1:D:264:LEU:HB3	1:D:275:PHE:CE1	2.54	0.42
1:D:47:ASP:HB3	1:D:57:LEU:HD13	2.02	0.42
1:C:329:TRP:CH2	1:C:369:VAL:CG1	2.95	0.41
1:C:177:GLY:HA3	3:C:1372:NAI:O5B	2.19	0.41
1:F:264:LEU:HB3	1:F:275:PHE:CE1	2.55	0.41
1:E:101[A]:ARG:HB2	1:E:101[A]:ARG:HE	1.54	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:222:ALA:O	1:C:226:GLU:HG3	2.20	0.41
1:E:51:LYS:HB2	1:E:51:LYS:HE3	1.80	0.41
1:A:356:ALA:CB	1:A:363:PHE:HB2	2.50	0.41
1:C:137:ALA:HB2	3:C:1372:NAI:H4N	2.01	0.41
1:F:175:GLY:O	1:F:180:GLY:HA3	2.21	0.41
1:E:267:ILE:O	3:E:1374:NAI:H2N	2.20	0.41
1:F:1:MET:SD	1:F:70:LEU:HB2	2.61	0.41
1:F:2:ARG:HE	1:F:2:ARG:HB2	1.69	0.41
1:C:1:MET:H3	1:C:31:HIS:HD2	1.68	0.41
1:E:140:LEU:HD22	1:F:150:MET:HE3	2.03	0.40

There are no symmetry-related clashes.

## 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	369/377 (98%)	362 (98%)	6 (2%)	1 (0%)	50	44
1	B	371/377 (98%)	364 (98%)	6 (2%)	1 (0%)	50	44
1	C	369/377 (98%)	361 (98%)	8 (2%)	0	100	100
1	D	368/377 (98%)	364 (99%)	4 (1%)	0	100	100
1	E	372/377 (99%)	366 (98%)	6 (2%)	0	100	100
1	F	373/377 (99%)	368 (99%)	5 (1%)	0	100	100
All	All	2222/2262 (98%)	2185 (98%)	35 (2%)	2 (0%)	59	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	272	GLY
1	B	272	GLY

### 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	276/282 (98%)	265 (96%)	11 (4%)	42	36
1	B	279/282 (99%)	273 (98%)	6 (2%)	64	65
1	C	276/282 (98%)	264 (96%)	12 (4%)	40	33
1	D	276/282 (98%)	270 (98%)	6 (2%)	64	65
1	E	279/282 (99%)	273 (98%)	6 (2%)	64	65
1	F	280/282 (99%)	274 (98%)	6 (2%)	66	67
All	All	1666/1692 (98%)	1619 (97%)	47 (3%)	56	54

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	70	LEU
1	A	71	LEU
1	A	143	GLN
1	A	212	CYS
1	A	249	LEU
1	A	290	VAL
1	A	293	THR
1	A	298	VAL
1	A	334	ARG
1	A	368	SER
1	B	57	LEU
1	B	71	LEU
1	B	130	LEU
1	B	284	ASP
1	B	293	THR
1	B	370	LEU
1	C	58	VAL
1	C	70	LEU
1	C	71	LEU
1	C	101	ARG
1	C	130	LEU
1	C	271	GLN

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Mol	Chain	Res	Type
1	C	290	VAL
1	C	293	THR
1	C	298	VAL
1	C	339	LEU
1	C	361	VAL
1	C	370	LEU
1	D	84	ARG
1	D	212	CYS
1	D	290	VAL
1	D	293	THR
1	D	298	VAL
1	D	357	THR
1	E	3	VAL
1	E	70	LEU
1	E	212	CYS
1	E	264	LEU
1	E	290	VAL
1	E	339	LEU
1	F	3	VAL
1	F	70	LEU
1	F	71	LEU
1	F	290	VAL
1	F	339	LEU
1	F	364	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	B	12	ASN
1	B	87	HIS
1	B	271	GLN
1	C	31	HIS
1	C	121	GLN
1	C	148	HIS
1	D	96	HIS
1	D	148	HIS
1	E	56	GLN
1	E	148	HIS
1	F	11	ASN
1	F	12	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	$\# Z  > 2$
3	NAI	A	1373	-	48,48,48	1.45	6 (12%)	73,73,73	1.92	14 (19%)
3	NAI	B	1372	-	48,48,48	1.44	6 (12%)	73,73,73	1.98	16 (21%)
3	NAI	C	1372	-	48,48,48	1.40	6 (12%)	73,73,73	1.93	12 (16%)
3	NAI	D	1371	-	48,48,48	1.46	6 (12%)	73,73,73	2.05	13 (17%)
3	NAI	E	1374	-	48,48,48	1.41	6 (12%)	73,73,73	1.72	12 (16%)
3	NAI	F	1374	-	48,48,48	1.40	6 (12%)	73,73,73	1.71	14 (19%)

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
3	NAI	A	1373	-	-	0/30/72/72	0/3/5/5
3	NAI	B	1372	-	-	0/30/72/72	0/3/5/5
3	NAI	C	1372	-	-	0/30/72/72	0/3/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAI	D	1371	-	-	0/30/72/72	0/3/5/5
3	NAI	E	1374	-	-	0/30/72/72	0/3/5/5
3	NAI	F	1374	-	-	0/30/72/72	0/3/5/5

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1373	NAI	C4N-C3N	-5.75	1.39	1.50
3	B	1372	NAI	C4N-C3N	-5.56	1.39	1.50
3	C	1372	NAI	C4N-C3N	-5.20	1.40	1.50
3	D	1371	NAI	C4N-C3N	-5.16	1.40	1.50
3	E	1374	NAI	C4N-C3N	-5.04	1.40	1.50
3	A	1373	NAI	C4N-C5N	-4.61	1.39	1.49
3	F	1374	NAI	C4N-C3N	-4.60	1.41	1.50
3	B	1372	NAI	C4N-C5N	-4.07	1.40	1.49
3	E	1374	NAI	C4N-C5N	-3.96	1.40	1.49
3	D	1371	NAI	C4N-C5N	-3.94	1.40	1.49
3	C	1372	NAI	C4N-C5N	-3.57	1.41	1.49
3	F	1374	NAI	C4N-C5N	-3.44	1.41	1.49
3	C	1372	NAI	C6N-C5N	3.38	1.40	1.33
3	D	1371	NAI	C6N-C5N	3.38	1.40	1.33
3	D	1371	NAI	C5A-C4A	3.33	1.48	1.40
3	E	1374	NAI	C5A-C4A	3.29	1.47	1.40
3	F	1374	NAI	C5A-C4A	3.28	1.47	1.40
3	E	1374	NAI	C6N-C5N	3.27	1.40	1.33
3	C	1372	NAI	C5A-C4A	3.21	1.47	1.40
3	F	1374	NAI	C6N-C5N	3.05	1.39	1.33
3	B	1372	NAI	C5A-C4A	3.02	1.47	1.40
3	B	1372	NAI	C4A-N9A	-2.76	1.33	1.37
3	C	1372	NAI	C2N-C3N	2.70	1.40	1.34
3	A	1373	NAI	C6N-C5N	2.69	1.39	1.33
3	D	1371	NAI	C2N-C3N	2.66	1.39	1.34
3	F	1374	NAI	C4A-N9A	-2.65	1.33	1.37
3	A	1373	NAI	C5A-C4A	2.59	1.46	1.40
3	E	1374	NAI	C2N-C3N	2.58	1.39	1.34
3	B	1372	NAI	C6N-C5N	2.54	1.38	1.33
3	E	1374	NAI	C4A-N9A	-2.48	1.34	1.37
3	B	1372	NAI	C2N-C3N	2.38	1.39	1.34
3	F	1374	NAI	C2N-C3N	2.34	1.39	1.34
3	A	1373	NAI	C4A-N9A	-2.29	1.34	1.37
3	C	1372	NAI	C4A-N9A	-2.27	1.34	1.37
3	D	1371	NAI	C4A-N9A	-2.26	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1373	NAI	C2N-C3N	2.17	1.39	1.34

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1371	NAI	O4B-C1B-N9A	8.64	116.47	108.44
3	C	1372	NAI	O4B-C1B-N9A	8.54	116.39	108.44
3	B	1372	NAI	O4B-C1B-N9A	7.98	115.86	108.44
3	A	1373	NAI	N3A-C2A-N1A	-7.39	122.53	128.71
3	E	1374	NAI	N3A-C2A-N1A	-7.03	122.83	128.71
3	A	1373	NAI	O4B-C1B-N9A	6.91	114.87	108.44
3	D	1371	NAI	N3A-C2A-N1A	-6.83	123.00	128.71
3	B	1372	NAI	N3A-C2A-N1A	-6.16	123.56	128.71
3	C	1372	NAI	N3A-C2A-N1A	-5.94	123.74	128.71
3	F	1374	NAI	N3A-C2A-N1A	-5.91	123.77	128.71
3	C	1372	NAI	N3A-C4A-N9A	5.50	135.37	125.43
3	E	1374	NAI	N3A-C4A-N9A	5.42	135.22	125.43
3	B	1372	NAI	N3A-C4A-N9A	5.26	134.93	125.43
3	A	1373	NAI	N3A-C4A-N9A	5.25	134.91	125.43
3	F	1374	NAI	N3A-C4A-N9A	5.20	134.83	125.43
3	D	1371	NAI	N3A-C4A-N9A	5.06	134.58	125.43
3	D	1371	NAI	O4D-C1D-N1N	4.93	118.50	108.05
3	E	1374	NAI	O4D-C1D-N1N	4.44	117.45	108.05
3	D	1371	NAI	C4B-O4B-C1B	-4.42	104.94	109.75
3	A	1373	NAI	C4B-O4B-C1B	-4.22	105.17	109.75
3	F	1374	NAI	O4D-C1D-N1N	4.12	116.78	108.05
3	F	1374	NAI	O4B-C1B-N9A	4.08	112.23	108.44
3	A	1373	NAI	C4A-C5A-N7A	-4.01	106.09	109.52
3	B	1372	NAI	C4B-O4B-C1B	-3.97	105.43	109.75
3	C	1372	NAI	O4D-C1D-N1N	3.83	116.15	108.05
3	B	1372	NAI	C4A-C5A-N7A	-3.82	106.25	109.52
3	D	1371	NAI	C4A-C5A-N7A	-3.75	106.31	109.52
3	E	1374	NAI	C8A-N9A-C4A	3.57	109.62	106.90
3	C	1372	NAI	C5A-C4A-N3A	-3.51	118.07	125.70
3	C	1372	NAI	C1D-N1N-C2N	-3.51	115.05	121.02
3	C	1372	NAI	C4A-C5A-N7A	-3.49	106.53	109.52
3	D	1371	NAI	C1D-N1N-C2N	-3.35	115.32	121.02
3	B	1372	NAI	C5A-C4A-N3A	-3.24	118.65	125.70
3	A	1373	NAI	C5A-C4A-N3A	-3.23	118.68	125.70
3	B	1372	NAI	PN-O3-PA	-3.20	122.30	131.68
3	E	1374	NAI	C4B-O4B-C1B	-3.17	106.31	109.75
3	B	1372	NAI	C4N-C3N-C2N	-3.13	117.87	121.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1372	NAI	C4B-O4B-C1B	-3.12	106.36	109.75
3	D	1371	NAI	C5A-C4A-N3A	-3.12	118.90	125.70
3	A	1373	NAI	C2A-N3A-C4A	3.07	122.76	114.01
3	F	1374	NAI	C1D-N1N-C2N	-3.05	115.82	121.02
3	B	1372	NAI	O4D-C1D-N1N	2.89	114.18	108.05
3	E	1374	NAI	C5A-C4A-N3A	-2.88	119.44	125.70
3	C	1372	NAI	C4N-C3N-C2N	-2.87	118.19	121.68
3	F	1374	NAI	C5A-C4A-N3A	-2.85	119.50	125.70
3	A	1373	NAI	C8A-N9A-C4A	2.82	109.05	106.90
3	C	1372	NAI	C2A-N3A-C4A	2.80	121.97	114.01
3	E	1374	NAI	C4A-C5A-N7A	-2.79	107.13	109.52
3	D	1371	NAI	C2A-N3A-C4A	2.72	121.75	114.01
3	A	1373	NAI	C1D-N1N-C2N	-2.66	116.49	121.02
3	D	1371	NAI	C3N-C7N-N7N	2.62	122.53	117.48
3	B	1372	NAI	C2A-N3A-C4A	2.57	121.33	114.01
3	B	1372	NAI	C5N-C4N-C3N	2.51	119.40	112.60
3	E	1374	NAI	O4D-C1D-C2D	-2.51	100.84	106.60
3	F	1374	NAI	C4A-C5A-N7A	-2.45	107.42	109.52
3	A	1373	NAI	O4D-C1D-N1N	2.45	113.24	108.05
3	B	1372	NAI	C1D-N1N-C2N	-2.45	116.85	121.02
3	B	1372	NAI	O4B-C1B-C2B	-2.42	103.06	106.77
3	E	1374	NAI	C2A-N3A-C4A	2.40	120.83	114.01
3	B	1372	NAI	C8A-N9A-C4A	2.39	108.73	106.90
3	F	1374	NAI	C8A-N9A-C4A	2.36	108.70	106.90
3	C	1372	NAI	PN-O3-PA	-2.32	124.88	131.68
3	C	1372	NAI	C5N-C4N-C3N	2.29	118.80	112.60
3	F	1374	NAI	C4N-C3N-C2N	-2.25	118.94	121.68
3	D	1371	NAI	C4N-C3N-C2N	-2.23	118.97	121.68
3	F	1374	NAI	PN-O3-PA	-2.22	125.17	131.68
3	F	1374	NAI	O2A-PA-O3	2.22	115.66	105.14
3	D	1371	NAI	PN-O3-PA	-2.19	125.27	131.68
3	E	1374	NAI	C1B-N9A-C4A	-2.19	122.86	126.64
3	A	1373	NAI	C5N-C4N-C3N	2.18	118.50	112.60
3	E	1374	NAI	C5N-C4N-C3N	2.17	118.47	112.60
3	B	1372	NAI	O4D-C1D-C2D	-2.16	101.64	106.60
3	D	1371	NAI	C5N-C4N-C3N	2.14	118.39	112.60
3	F	1374	NAI	C5N-C4N-C3N	2.10	118.29	112.60
3	E	1374	NAI	O4B-C1B-N9A	2.09	110.38	108.44
3	F	1374	NAI	N6A-C6A-N1A	2.09	123.46	119.36
3	F	1374	NAI	C2A-N1A-C6A	2.05	122.48	118.77
3	A	1373	NAI	O4D-C1D-C2D	-2.04	101.92	106.60
3	B	1372	NAI	O5B-PA-O1A	-2.02	101.45	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1373	NAI	O2A-PA-O3	2.01	114.69	105.14
3	A	1373	NAI	O4B-C1B-C2B	-2.00	103.70	106.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	371/377 (98%)	0.51	16 (4%) 34 32	26, 46, 56, 68	0
1	B	370/377 (98%)	0.16	4 (1%) 77 78	25, 40, 51, 58	0
1	C	371/377 (98%)	0.57	29 (7%) 13 12	26, 47, 61, 70	0
1	D	370/377 (98%)	0.14	5 (1%) 72 72	25, 40, 52, 57	0
1	E	373/377 (98%)	0.76	34 (9%) 9 9	27, 50, 65, 76	0
1	F	373/377 (98%)	0.45	16 (4%) 34 32	26, 42, 49, 66	0
All	All	2228/2262 (98%)	0.43	104 (4%) 30 29	25, 44, 57, 76	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	283	TYR	5.8
1	E	372	HIS	4.8
1	C	371	ALA	4.2
1	A	57	LEU	4.2
1	F	34	LEU	4.1
1	C	363	PHE	4.0
1	C	356	ALA	3.9
1	C	243	GLY	3.8
1	F	373	HIS	3.8
1	C	368	SER	3.6
1	C	359	LEU	3.6
1	C	362	PRO	3.5
1	C	361	VAL	3.5
1	E	373	HIS	3.5
1	C	358	ASP	3.4
1	A	283	TYR	3.4
1	C	360	GLY	3.4
1	F	186	ILE	3.3
1	E	186	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	371	ALA	3.3
1	C	357	THR	3.3
1	E	37	ALA	3.3
1	F	207	LEU	3.2
1	E	61	ALA	3.2
1	C	355	VAL	3.2
1	D	368	SER	3.2
1	E	34	LEU	3.0
1	C	257	HIS	3.0
1	F	194	VAL	2.9
1	F	187	ALA	2.9
1	C	292	ASP	2.9
1	E	189	GLY	2.9
1	E	366	PRO	2.9
1	C	353	GLU	2.8
1	C	364	THR	2.8
1	B	14	PHE	2.8
1	E	46	THR	2.8
1	B	283	TYR	2.8
1	E	183	ALA	2.8
1	E	187	ALA	2.8
1	A	14	PHE	2.8
1	A	365	GLU	2.7
1	F	184	ALA	2.7
1	E	82	TYR	2.7
1	A	51	LYS	2.7
1	A	38	GLY	2.7
1	A	368	SER	2.6
1	F	372	HIS	2.6
1	E	56	GLN	2.6
1	C	30	GLY	2.5
1	C	365	GLU	2.5
1	A	215	ILE	2.5
1	E	83	GLY	2.5
1	E	215	ILE	2.5
1	E	53	ALA	2.5
1	F	181	TYR	2.5
1	E	171	VAL	2.5
1	E	142	ALA	2.4
1	F	57	LEU	2.4
1	E	78	ILE	2.4
1	D	209	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	370	LEU	2.4
1	C	285	HIS	2.4
1	E	207	LEU	2.4
1	E	370	LEU	2.4
1	D	243	GLY	2.4
1	C	2	ARG	2.4
1	E	85	LEU	2.4
1	C	215	ILE	2.4
1	C	281	THR	2.3
1	C	282	THR	2.3
1	F	215	ILE	2.3
1	E	104	THR	2.3
1	F	196	VAL	2.3
1	E	192	ALA	2.3
1	A	370	LEU	2.3
1	A	45	ILE	2.3
1	E	79	ALA	2.3
1	E	51	LYS	2.3
1	A	58	VAL	2.2
1	C	354	ARG	2.2
1	E	256	ALA	2.2
1	C	242	PRO	2.2
1	E	65	TRP	2.2
1	A	32	GLU	2.2
1	C	256	ALA	2.2
1	F	183	ALA	2.2
1	A	37	ALA	2.2
1	A	285	HIS	2.2
1	F	189	GLY	2.2
1	E	367	ALA	2.2
1	F	173	VAL	2.2
1	E	329	TRP	2.1
1	C	57	LEU	2.1
1	B	186	ILE	2.1
1	E	176	ALA	2.1
1	E	178	THR	2.1
1	E	64	VAL	2.1
1	F	38	GLY	2.1
1	E	234	LEU	2.0
1	D	245	LYS	2.0
1	A	363	PHE	2.0
1	D	361	VAL	2.0

*Continued on next page...*

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Mol	Chain	Res	Type	RSRZ
1	B	212	CYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains

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

## 6.3 Carbohydrates

There are no carbohydrates in this entry.

## 6.4 Ligands

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAI	C	1372	44/44	0.13	-0.20	36,41,46,47	0
3	NAI	D	1371	44/44	0.10	-0.84	30,34,39,43	0
3	NAI	A	1373	44/44	0.09	-1.51	30,34,39,43	0
3	NAI	E	1374	44/44	0.10	-1.52	27,31,40,41	0
3	NAI	F	1374	44/44	0.10	-1.76	20,24,29,31	0
3	NAI	B	1372	44/44	0.07	-2.10	23,29,33,36	0
2	MG	B	1371	1/1	0.03	-2.24	45,45,45,45	0
2	MG	A	1372	1/1	0.11	-2.58	48,48,48,48	0

## 6.5 Other polymers

There are no such residues in this entry.