



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:47 AM GMT

PDB ID : 2IOD
Title : Binding of two substrate analogue molecules to dihydroflavonol-4-reductase alters the functional geometry of the catalytic site
Authors : Petit, P.; Langlois d'Estaintot, B.; Granier, T.; Gallois, B.
Deposited on : 2006-10-10
Resolution : 2.06 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 (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

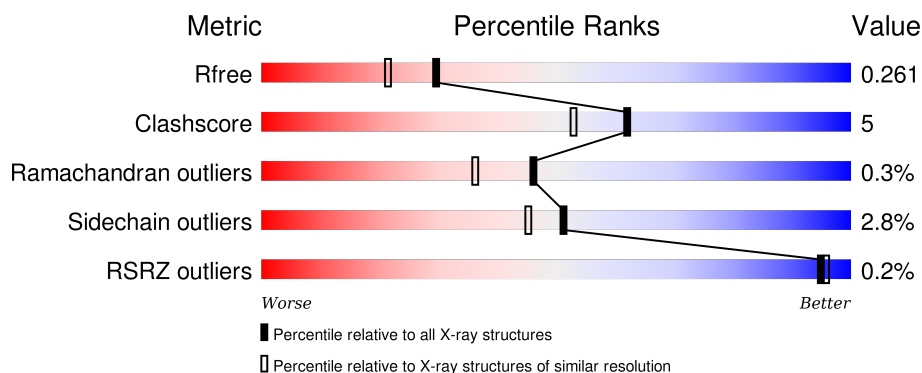
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.06 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	1799 (2.08-2.04)
Clashscore	102246	1910 (2.08-2.04)
Ramachandran outliers	100387	1893 (2.08-2.04)
Sidechain outliers	100360	1893 (2.08-2.04)
RSRZ outliers	91569	1802 (2.08-2.04)

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	337	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 18%, green 76%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 76% 18% • 5% </div> </div>
1	B	337	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 82%, yellow 14%, grey 4%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 82% 14% • • </div> </div>
1	C	337	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 87%, yellow 9%, grey 4%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 87% 9% • </div> </div>
1	D	337	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 86%, yellow 9%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 86% 9% 5% </div> </div>

2 Entry composition [i](#)

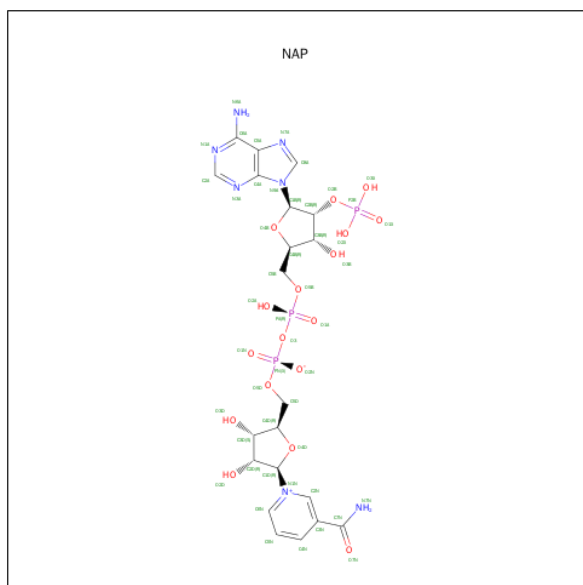
There are 4 unique types of molecules in this entry. The entry contains 11125 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Dihydroflavonol 4-reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	2	0
			2477	1588	412	457	20			
1	B	326	Total	C	N	O	S	0	2	0
			2511	1608	415	466	22			
1	C	325	Total	C	N	O	S	0	1	0
			2509	1606	413	469	21			
1	D	321	Total	C	N	O	S	0	1	0
			2484	1590	410	463	21			

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



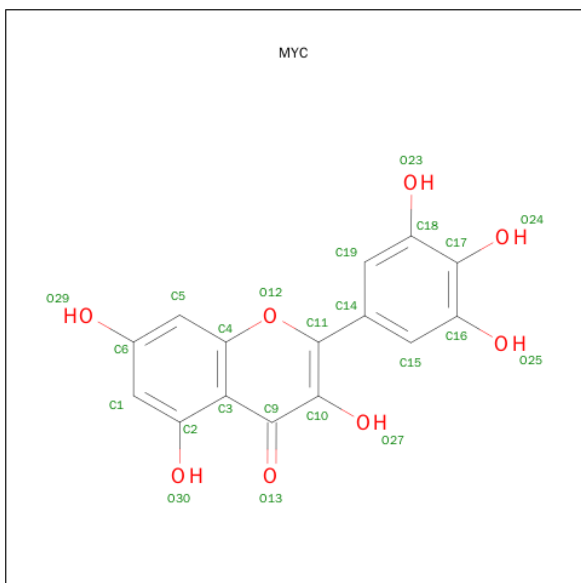
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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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 3,5,7-TRIHydroxy-2-(3,4,5-TRIHydroxyphenyl)-4H-CHROMEN-4-ONE (three-letter code: MYC) (formula: C₁₅H₁₀O₈).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			23	15	8		
3	A	1	Total	C	O	0	0
			23	15	8		
3	B	1	Total	C	O	0	0
			23	15	8		
3	B	1	Total	C	O	0	0
			23	15	8		
3	C	1	Total	C	O	0	0
			23	15	8		
3	C	1	Total	C	O	0	0
			23	15	8		
3	D	1	Total	C	O	0	0
			23	15	8		
3	D	1	Total	C	O	0	0
			23	15	8		

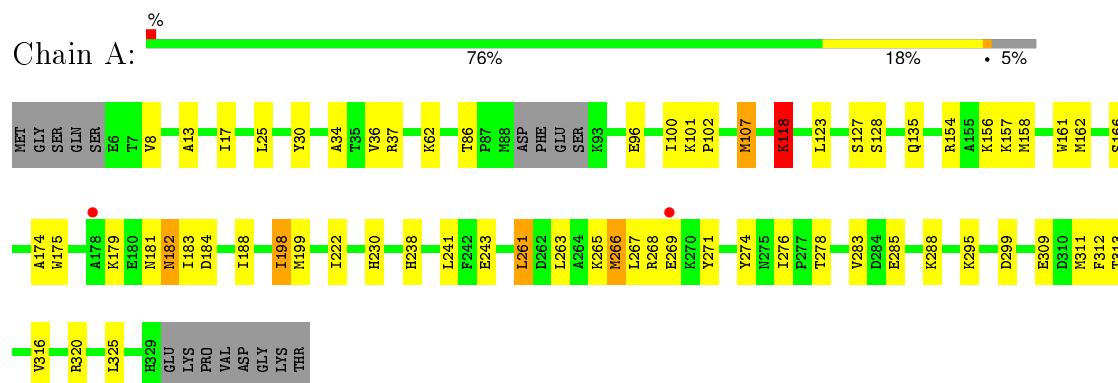
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	151	Total 151	O 151	0	0
4	B	174	Total 174	O 174	0	0
4	C	201	Total 201	O 201	0	0
4	D	242	Total 242	O 242	0	0

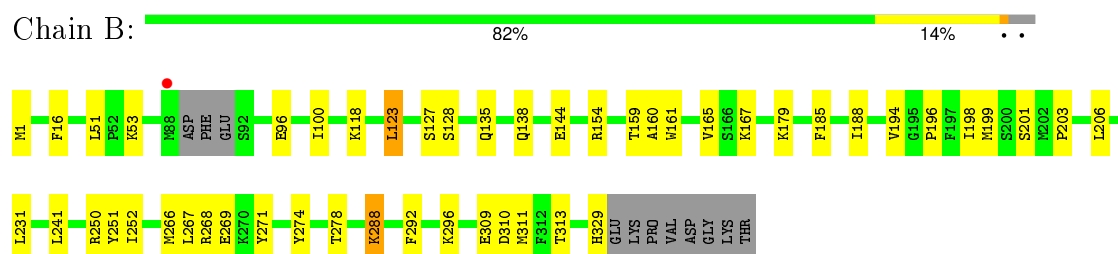
3 Residue-property plots [i](#)

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

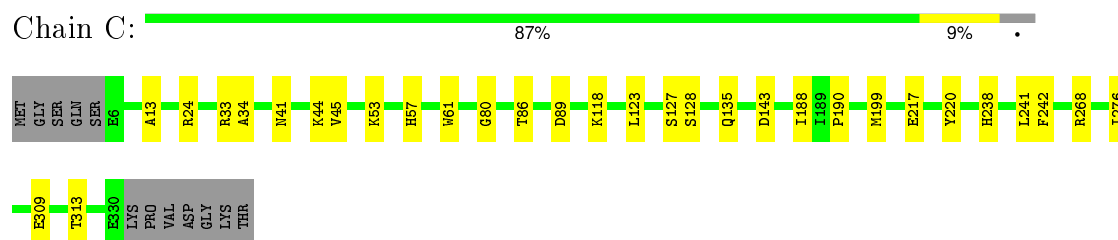
- Molecule 1: Dihydroflavonol 4-reductase



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- Molecule 1: Dihydroflavonol 4-reductase



L300	E309	T313	G314	A315	H329	GLU	LYS	PRO	VAL	ASP	GLY	LYS	THR	MET	GLY	SER	GLN	SER	ASP	PHE	GLU	S92	L123	S127	S128	Q135	R154	K157	M158	T159	I188	I198	M199	L206	S211	P212	H238	Y251	I262	R268	I276	K288	S289	F292
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	47.23Å 177.96Å 92.60Å 90.00° 104.77° 90.00°	Depositor
Resolution (Å)	89.44 – 2.06 89.54 – 2.06	Depositor EDS
% Data completeness (in resolution range)	98.9 (89.44-2.06) 98.9 (89.54-2.06)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.07Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.189 , 0.257 0.195 , 0.261	Depositor DCC
R_{free} test set	4501 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	29.8	Xtriage
Anisotropy	0.590	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 55.9	EDS
Estimated twinning fraction	0.170 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 89895 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11125	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.66	0/2539	0.89	2/3450 (0.1%)
1	B	0.64	0/2573	0.87	0/3494
1	C	0.65	0/2568	0.85	2/3490 (0.1%)
1	D	0.69	0/2542	0.90	1/3453 (0.0%)
All	All	0.66	0/10222	0.88	5/13887 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	D	24	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	C	143	ASP	CB-CG-OD1	5.76	123.48	118.30
1	A	107	MET	CG-SD-CE	5.36	108.78	100.20
1	C	24	ARG	NE-CZ-NH1	5.05	122.83	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2477	0	2431	42	0
1	B	2511	0	2457	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2509	0	2447	19	0
1	D	2484	0	2432	16	0
2	A	48	0	25	2	0
2	B	48	0	25	1	0
2	C	48	0	25	4	0
2	D	48	0	25	2	0
3	A	46	0	11	2	0
3	B	46	0	11	4	0
3	C	46	0	15	2	0
3	D	46	0	10	1	0
4	A	151	0	0	3	0
4	B	174	0	0	1	0
4	C	201	0	0	3	0
4	D	242	0	0	1	0
All	All	11125	0	9914	109	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 5.

All (109) 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:D:309:GLU:O	1:D:313[B]:THR:HG22	1.65	0.95
1:A:312:PHE:O	1:A:316:VAL:HG23	1.81	0.80
1:D:199:MET:HE3	4:D:4522:HOH:O	1.92	0.69
1:A:17:ILE:HD12	2:A:1340:NAP:H51N	1.82	0.61
1:A:263:LEU:HD12	1:A:266:MET:HE2	1.82	0.61
1:D:309:GLU:O	1:D:313[A]:THR:HG23	2.01	0.60
1:B:16:PHE:CE1	1:B:231:LEU:HD22	2.37	0.60
1:A:175:TRP:O	1:A:179:LYS:HD3	2.02	0.59
1:B:309:GLU:O	1:B:313[A]:THR:HG23	2.04	0.58
1:A:8:VAL:HG21	1:A:25:LEU:HD13	1.86	0.58
1:A:182:ASN:HD21	1:D:159:THR:H	1.52	0.57
1:B:161:TRP:O	1:B:165:VAL:HG23	2.05	0.56
1:C:199:MET:HE1	4:C:3439:HOH:O	2.07	0.55
1:A:128:SER:HG	3:A:1342:MYC:HO3	1.54	0.55
1:B:96:GLU:OE2	1:B:154:ARG:NH1	2.39	0.55
1:B:128:SER:HG	3:B:2342:MYC:HO3	1.55	0.54
1:B:196:PRO:O	1:B:231:LEU:HD23	2.08	0.54
1:A:285:GLU:CB	4:A:1477:HOH:O	2.54	0.54
1:A:96:GLU:OE2	1:A:154:ARG:NH1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:SER:OG	3:A:1342:MYC:O23	2.26	0.53
1:A:265:LYS:O	1:A:269:GLU:OE1	2.26	0.53
1:C:199:MET:HE3	4:C:3390:HOH:O	2.09	0.53
1:A:271:TYR:CE2	1:A:316:VAL:HG21	2.44	0.52
1:A:316:VAL:HG13	1:A:325:LEU:CD1	2.40	0.52
1:D:37:ARG:NE	2:D:4340:NAP:O3X	2.40	0.52
1:C:128:SER:OG	3:C:3342:MYC:O23	2.28	0.51
1:D:188:ILE:CD1	1:D:238:HIS:HA	2.39	0.51
1:D:268:ARG:HG2	1:D:276:ILE:HB	1.93	0.51
1:A:188:ILE:CD1	1:A:241:LEU:HD12	2.41	0.51
1:C:190:PRO:HG2	2:C:3340:NAP:C6N	2.40	0.51
1:A:157:LYS:HE3	1:A:161:TRP:CZ2	2.46	0.51
1:B:96:GLU:HA	1:B:100:ILE:HD12	1.94	0.50
1:A:261:LEU:HD13	1:A:283:VAL:HG11	1.94	0.50
1:B:267:LEU:O	1:B:271:TYR:N	2.39	0.50
1:D:13:ALA:CB	1:D:34:ALA:HB1	2.42	0.49
1:C:309:GLU:O	1:C:313[B]:THR:HG22	2.12	0.49
1:A:8:VAL:CG2	1:A:25:LEU:HD13	2.42	0.49
1:A:309:GLU:O	1:A:313[A]:THR:HG23	2.13	0.49
1:B:138:GLN:O	1:B:288:LYS:NZ	2.43	0.49
1:A:127:SER:O	2:A:1340:NAP:H6N	2.12	0.49
1:A:13:ALA:CB	1:A:34:ALA:HB1	2.43	0.49
1:C:53:LYS:HE2	1:C:57:HIS:CD2	2.48	0.48
1:B:144:GLU:HG2	1:B:250:ARG:O	2.13	0.48
1:B:53:LYS:HD2	4:B:2493:HOH:O	2.12	0.48
1:A:188:ILE:CD1	1:A:238:HIS:HA	2.44	0.48
1:C:309:GLU:O	1:C:313[B]:THR:CG2	2.61	0.47
1:A:184:ASP:OD1	1:A:184:ASP:C	2.50	0.47
1:A:316:VAL:HG13	1:A:325:LEU:HD12	1.95	0.47
3:C:3342:MYC:O23	4:C:3519:HOH:O	2.21	0.47
1:A:268:ARG:HA	1:A:276:ILE:HD12	1.97	0.47
1:C:190:PRO:HG2	2:C:3340:NAP:C5N	2.46	0.46
1:A:30:TYR:OH	1:A:243:GLU:OE2	2.21	0.46
1:C:188:ILE:HD13	1:C:241:LEU:HD12	1.97	0.46
1:C:217:GLU:HG2	1:C:220:TYR:CE2	2.50	0.46
1:B:123:LEU:HD13	1:B:185:PHE:CD1	2.50	0.46
1:C:44:LYS:NZ	2:C:3340:NAP:O1X	2.37	0.46
1:B:188:ILE:HG12	1:B:241:LEU:HD12	1.97	0.46
1:A:188:ILE:HD11	1:A:241:LEU:HD12	1.96	0.46
1:B:266:MET:CE	1:B:267:LEU:HD23	2.46	0.46
1:D:251:TYR:OH	1:D:300:LEU:HD11	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:ALA:CB	1:C:34:ALA:HB1	2.46	0.46
1:C:41:ASN:O	1:C:45:VAL:HG22	2.16	0.45
1:A:266:MET:HE3	1:A:267:LEU:HG	1.98	0.45
1:A:107:MET:HG2	1:A:174:ALA:HB2	1.98	0.45
1:A:230:HIS:HD2	1:A:311:MET:HA	1.82	0.45
1:A:157:LYS:HE3	1:A:161:TRP:CE2	2.52	0.45
1:B:251:TYR:CZ	1:B:296:LYS:HE2	2.51	0.45
1:B:199:MET:HE2	1:B:201:SER:O	2.17	0.45
1:C:188:ILE:CD1	1:C:241:LEU:HD12	2.46	0.45
1:B:252:ILE:HG21	1:B:292:PHE:HB3	1.99	0.44
1:D:252:ILE:HG21	1:D:292:PHE:HB3	1.99	0.44
1:B:199:MET:CE	1:B:201:SER:O	2.65	0.44
1:D:154:ARG:O	1:D:157:LYS:HE3	2.16	0.44
1:A:162:MET:O	1:A:166:SER:HB3	2.17	0.44
1:B:199:MET:HE1	1:B:203:PRO:HA	2.00	0.44
1:B:167:LYS:HG3	3:B:2342:MYC:O24	2.18	0.43
1:B:268:ARG:CZ	1:B:278:THR:HA	2.49	0.43
1:A:36:VAL:O	1:A:62:LYS:HA	2.19	0.43
1:B:266:MET:HE1	1:B:267:LEU:HD23	2.01	0.43
1:B:271:TYR:OH	1:B:313[A]:THR:HA	2.19	0.43
1:C:268:ARG:HG2	1:C:276:ILE:HB	2.00	0.43
1:A:295:LYS:NZ	1:A:299:ASP:OD2	2.51	0.43
1:B:194:VAL:HG13	1:B:206:LEU:CD2	2.48	0.43
1:C:188:ILE:CD1	1:C:238:HIS:HA	2.49	0.42
1:D:288:LYS:HG2	1:D:289:SER:O	2.19	0.42
1:B:51:LEU:HD21	1:B:198:ILE:CD1	2.48	0.42
1:B:271:TYR:OH	1:B:313[B]:THR:HA	2.19	0.42
1:B:310:ASP:O	1:B:311:MET:C	2.57	0.42
1:B:274:TYR:HD1	1:B:329:HIS:ND1	2.16	0.42
1:A:118:LYS:NZ	4:A:1358:HOH:O	2.53	0.42
1:B:159:THR:O	1:B:160:ALA:HB3	2.20	0.41
1:D:206:LEU:HD13	1:D:315:ALA:HB1	2.00	0.41
1:A:101:LYS:HB3	1:A:102:PRO:HD3	2.02	0.41
1:A:230:HIS:CD2	1:A:311:MET:HA	2.56	0.41
1:A:179:LYS:HE2	4:A:1493:HOH:O	2.20	0.41
1:A:181:ASN:O	1:A:183:ILE:N	2.54	0.41
3:B:2342:MYC:O27	3:B:2342:MYC:H15	2.21	0.41
1:D:127:SER:O	2:D:4340:NAP:H6N	2.21	0.41
1:B:127:SER:O	2:B:2340:NAP:H6N	2.20	0.41
1:B:160:ALA:HB2	3:B:2342:MYC:C4	2.50	0.41
1:A:96:GLU:HA	1:A:100:ILE:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:TYR:OH	1:A:320:ARG:NE	2.47	0.41
1:D:211:SER:N	1:D:212:PRO:CD	2.84	0.41
1:C:80:GLY:HA3	1:C:242:PHE:CE1	2.56	0.40
1:A:198:ILE:HG21	1:A:198:ILE:HD13	1.82	0.40
1:A:268:ARG:HG2	1:A:276:ILE:HB	2.02	0.40
1:D:128:SER:OG	3:D:4342:MYC:O25	2.36	0.40
1:C:127:SER:O	2:C:3340:NAP:H6N	2.20	0.40
1:C:33:ARG:HD3	1:C:61:TRP:CZ2	2.56	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	318/337 (94%)	302 (95%)	14 (4%)	2 (1%)	30	17
1	B	324/337 (96%)	308 (95%)	15 (5%)	1 (0%)	46	36
1	C	324/337 (96%)	316 (98%)	7 (2%)	1 (0%)	46	36
1	D	318/337 (94%)	307 (96%)	11 (4%)	0	100	100
All	All	1284/1348 (95%)	1233 (96%)	47 (4%)	4 (0%)	46	36

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	182	ASN
1	A	118	LYS
1	B	118	LYS
1	C	118	LYS

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	267/293 (91%)	254 (95%)	13 (5%)	31	21
1	B	269/293 (92%)	263 (98%)	6 (2%)	60	55
1	C	269/293 (92%)	265 (98%)	4 (2%)	72	70
1	D	268/293 (92%)	261 (97%)	7 (3%)	54	48
All	All	1073/1172 (92%)	1043 (97%)	30 (3%)	51	45

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	THR
1	A	118	LYS
1	A	123	LEU
1	A	135	GLN
1	A	156	LYS
1	A	158	MET
1	A	198	ILE
1	A	199	MET
1	A	222	ILE
1	A	261	LEU
1	A	266	MET
1	A	278	THR
1	A	288	LYS
1	B	1	MET
1	B	123	LEU
1	B	135	GLN
1	B	179	LYS
1	B	269	GLU
1	B	288	LYS
1	C	86	THR
1	C	89	ASP
1	C	123	LEU
1	C	135	GLN
1	D	86	THR

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Mol	Chain	Res	Type
1	D	92	SER
1	D	123	LEU
1	D	135	GLN
1	D	158	MET
1	D	198	ILE
1	D	288	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	HIS
1	A	133	ASN
1	A	182	ASN
1	A	230	HIS
1	A	236	ASN
1	A	275	ASN
1	B	57	HIS
1	B	236	ASN
1	C	57	HIS
1	C	236	ASN
1	C	275	ASN
1	D	133	ASN
1	D	138	GLN
1	D	181	ASN
1	D	236	ASN
1	D	275	ASN

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 ⓘ

12 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	1340	-	42,52,52	1.56	4 (9%)	54,80,80	2.17	11 (20%)
3	MYC	A	1341	-	21,25,25	1.59	2 (9%)	29,38,38	1.39	4 (13%)
3	MYC	A	1342	-	21,25,25	1.78	3 (14%)	29,38,38	1.68	5 (17%)
2	NAP	B	2340	-	42,52,52	1.57	3 (7%)	54,80,80	2.57	14 (25%)
3	MYC	B	2341	-	21,25,25	1.75	2 (9%)	29,38,38	1.34	5 (17%)
3	MYC	B	2342	-	21,25,25	1.60	3 (14%)	29,38,38	1.49	6 (20%)
2	NAP	C	3340	-	42,52,52	1.52	2 (4%)	54,80,80	2.37	6 (11%)
3	MYC	C	3341	-	21,25,25	1.69	3 (14%)	29,38,38	1.51	6 (20%)
3	MYC	C	3342	-	21,25,25	1.40	3 (14%)	29,38,38	2.16	11 (37%)
2	NAP	D	4340	-	42,52,52	1.48	4 (9%)	54,80,80	2.68	11 (20%)
3	MYC	D	4341	-	21,25,25	1.73	1 (4%)	29,38,38	1.34	3 (10%)
3	MYC	D	4342	-	21,25,25	1.59	6 (28%)	29,38,38	1.94	9 (31%)

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	1340	-	-	0/27/67/67	0/5/5/5
3	MYC	A	1341	-	-	0/4/4/4	0/3/3/3
3	MYC	A	1342	-	-	0/4/4/4	0/3/3/3
2	NAP	B	2340	-	-	0/27/67/67	0/5/5/5
3	MYC	B	2341	-	-	0/4/4/4	0/3/3/3
3	MYC	B	2342	-	-	0/4/4/4	0/3/3/3
2	NAP	C	3340	-	-	0/27/67/67	0/5/5/5
3	MYC	C	3341	-	-	0/4/4/4	0/3/3/3
3	MYC	C	3342	-	-	0/4/4/4	0/3/3/3
2	NAP	D	4340	-	-	0/27/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MYC	D	4341	-	-	0/4/4/4	0/3/3/3
3	MYC	D	4342	-	-	0/4/4/4	0/3/3/3

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3342	MYC	C18-C17	-3.79	1.35	1.39
2	A	1340	NAP	O4D-C4D	-2.97	1.38	1.45
3	D	4342	MYC	C16-C17	-2.74	1.36	1.39
3	D	4342	MYC	C18-C17	-2.59	1.36	1.39
3	A	1342	MYC	C18-C17	-2.49	1.37	1.39
3	B	2342	MYC	C18-C17	-2.33	1.37	1.39
2	D	4340	NAP	C3N-C7N	-2.30	1.46	1.50
2	B	2340	NAP	PN-O2N	-2.19	1.45	1.54
3	C	3341	MYC	C2-C3	-2.12	1.39	1.43
3	D	4342	MYC	C3-C4	-2.11	1.38	1.41
3	D	4342	MYC	C2-C3	-2.02	1.39	1.43
2	D	4340	NAP	C2A-N1A	2.05	1.37	1.33
3	A	1341	MYC	C14-C11	2.16	1.49	1.46
2	A	1340	NAP	C2A-N1A	2.27	1.38	1.33
3	B	2341	MYC	C14-C11	2.38	1.49	1.46
3	C	3341	MYC	C14-C11	2.51	1.49	1.46
2	C	3340	NAP	C2A-N3A	2.59	1.36	1.32
3	C	3342	MYC	C14-C11	2.65	1.49	1.46
3	B	2342	MYC	C14-C11	2.75	1.50	1.46
3	D	4342	MYC	C14-C11	2.91	1.50	1.46
2	D	4340	NAP	C2A-N3A	3.01	1.37	1.32
3	A	1342	MYC	C14-C11	3.03	1.50	1.46
2	A	1340	NAP	C2A-N3A	3.05	1.37	1.32
3	C	3342	MYC	C9-C3	3.34	1.45	1.41
2	B	2340	NAP	C2A-N3A	3.46	1.38	1.32
3	D	4342	MYC	C9-C3	4.22	1.47	1.41
3	B	2342	MYC	C9-C3	5.53	1.49	1.41
3	A	1342	MYC	C9-C3	6.09	1.49	1.41
3	C	3341	MYC	C9-C3	6.10	1.49	1.41
3	A	1341	MYC	C9-C3	6.21	1.49	1.41
3	D	4341	MYC	C9-C3	6.52	1.50	1.41
2	D	4340	NAP	O7N-C7N	6.56	1.38	1.24
3	B	2341	MYC	C9-C3	6.61	1.50	1.41
2	B	2340	NAP	O7N-C7N	7.28	1.39	1.24
2	A	1340	NAP	O7N-C7N	7.44	1.40	1.24
2	C	3340	NAP	O7N-C7N	7.67	1.40	1.24

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	4340	NAP	N3A-C2A-N1A	-14.55	117.75	128.89
2	C	3340	NAP	N3A-C2A-N1A	-13.62	118.47	128.89
2	B	2340	NAP	N3A-C2A-N1A	-11.57	120.04	128.89
2	A	1340	NAP	N3A-C2A-N1A	-9.70	121.47	128.89
2	B	2340	NAP	O7N-C7N-C3N	-5.15	113.97	119.59
2	B	2340	NAP	C1B-N9A-C4A	-5.04	119.34	126.94
2	D	4340	NAP	C4B-O4B-C1B	-4.87	104.36	109.72
2	D	4340	NAP	O7N-C7N-C3N	-4.75	114.40	119.59
2	D	4340	NAP	C1B-N9A-C4A	-4.68	119.88	126.94
2	A	1340	NAP	C4B-O4B-C1B	-4.66	104.60	109.72
2	A	1340	NAP	O7N-C7N-C3N	-4.61	114.55	119.59
2	C	3340	NAP	C4B-O4B-C1B	-4.45	104.83	109.72
2	C	3340	NAP	C1B-N9A-C4A	-4.32	120.43	126.94
2	B	2340	NAP	O3X-P2B-O1X	-4.20	97.07	110.58
3	C	3342	MYC	O24-C17-C18	-3.88	109.78	119.63
3	C	3342	MYC	C14-C19-C18	-3.36	118.14	120.98
2	B	2340	NAP	O3-PA-O5B	-3.27	94.27	102.94
3	A	1341	MYC	C1-C2-C3	-3.17	118.11	120.84
2	A	1340	NAP	O3-PN-O5D	-3.16	94.55	102.94
3	C	3342	MYC	O23-C18-C17	-3.16	109.69	117.91
3	A	1341	MYC	C6-C5-C4	-3.04	117.62	120.42
2	B	2340	NAP	C3N-C2N-N1N	-2.96	116.95	120.36
3	C	3342	MYC	C1-C2-C3	-2.94	118.31	120.84
3	D	4342	MYC	O25-C16-C17	-2.92	110.32	117.91
3	A	1342	MYC	C19-C18-C17	-2.91	118.63	120.42
3	C	3341	MYC	C10-C9-C3	-2.86	117.12	121.25
2	A	1340	NAP	O4D-C1D-N1N	-2.80	105.05	108.13
3	D	4342	MYC	C14-C15-C16	-2.77	118.64	120.98
2	B	2340	NAP	C4A-C5A-N7A	-2.67	107.02	109.48
3	B	2341	MYC	C14-C15-C16	-2.62	118.76	120.98
2	C	3340	NAP	O3X-P2B-O2X	-2.60	97.46	107.38
3	D	4342	MYC	O24-C17-C16	-2.59	113.06	119.63
3	D	4342	MYC	O12-C4-C3	-2.57	118.50	121.15
2	D	4340	NAP	C5N-C4N-C3N	-2.41	117.31	120.33
2	B	2340	NAP	C4B-O4B-C1B	-2.31	107.18	109.72
3	C	3342	MYC	C14-C15-C16	-2.25	119.08	120.98
3	D	4341	MYC	O29-C6-C5	-2.24	114.23	121.04
3	C	3341	MYC	C11-O12-C4	-2.23	119.17	122.30
3	C	3341	MYC	C14-C19-C18	-2.16	119.15	120.98
3	A	1341	MYC	C10-C9-C3	-2.14	118.16	121.25
3	A	1342	MYC	C14-C15-C16	-2.14	119.17	120.98
3	B	2341	MYC	C10-C9-C3	-2.13	118.17	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2342	MYC	C19-C18-C17	-2.12	119.11	120.42
3	C	3341	MYC	C19-C18-C17	-2.05	119.16	120.42
2	D	4340	NAP	O3X-P2B-O1X	-2.02	104.08	110.58
3	C	3342	MYC	C15-C16-C17	-2.02	119.18	120.42
2	A	1340	NAP	O4B-C1B-N9A	2.07	112.44	108.10
3	D	4342	MYC	C11-O12-C4	2.09	125.24	122.30
3	B	2342	MYC	C2-C3-C4	2.10	120.48	117.84
2	A	1340	NAP	O2N-PN-O1N	2.10	123.89	112.53
3	A	1341	MYC	C14-C11-C10	2.11	124.05	120.04
3	B	2342	MYC	O23-C18-C19	2.13	125.15	119.42
2	A	1340	NAP	O2A-PA-O1A	2.16	124.23	112.53
3	B	2341	MYC	C15-C16-C17	2.18	121.77	120.42
3	B	2341	MYC	C14-C11-C10	2.21	124.23	120.04
3	B	2341	MYC	O12-C4-C5	2.21	119.00	116.18
2	B	2340	NAP	O2N-PN-O5D	2.25	119.80	108.46
2	B	2340	NAP	C2D-C3D-C4D	2.27	107.27	102.61
3	D	4341	MYC	O12-C4-C5	2.31	119.13	116.18
2	D	4340	NAP	O5B-PA-O1A	2.37	118.81	109.62
2	A	1340	NAP	C4D-O4D-C1D	2.39	112.34	109.72
2	D	4340	NAP	P2B-O2B-C2B	2.47	127.48	121.56
2	D	4340	NAP	C3N-C7N-N7N	2.54	120.60	117.82
3	B	2342	MYC	O12-C4-C5	2.55	119.43	116.18
2	C	3340	NAP	C2A-N1A-C6A	2.68	123.56	118.77
2	B	2340	NAP	O2X-P2B-O1X	2.70	119.28	110.58
3	B	2342	MYC	C14-C11-C10	2.76	125.28	120.04
3	D	4342	MYC	O24-C17-C18	2.77	126.66	119.63
3	C	3342	MYC	C2-C3-C4	2.79	121.35	117.84
3	C	3341	MYC	O12-C4-C5	2.93	119.91	116.18
3	A	1342	MYC	O23-C18-C19	2.95	127.37	119.42
3	A	1342	MYC	C18-C17-C16	3.05	121.22	119.55
3	C	3341	MYC	C18-C17-C16	3.07	121.23	119.55
3	B	2342	MYC	C18-C17-C16	3.11	121.25	119.55
2	B	2340	NAP	C2N-C3N-C4N	3.21	121.86	118.29
2	D	4340	NAP	C2N-C3N-C4N	3.24	121.89	118.29
3	D	4342	MYC	O25-C16-C15	3.24	128.14	119.42
3	C	3342	MYC	C14-C11-C10	3.32	126.35	120.04
3	C	3342	MYC	O24-C17-C16	3.35	128.12	119.63
2	C	3340	NAP	O2X-P2B-O1X	3.51	121.88	110.58
2	A	1340	NAP	C3N-C7N-N7N	3.72	121.89	117.82
3	D	4342	MYC	O12-C4-C5	3.75	120.96	116.18
2	A	1340	NAP	O2X-P2B-O1X	3.76	122.68	110.58
3	C	3342	MYC	O23-C18-C19	3.76	129.55	119.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4341	MYC	O12-C11-C14	4.11	118.99	113.14
3	A	1342	MYC	C14-C11-C10	4.45	128.49	120.04
3	C	3342	MYC	C18-C17-C16	4.58	122.06	119.55
3	D	4342	MYC	C14-C11-C10	4.93	129.40	120.04
2	D	4340	NAP	O2X-P2B-O1X	5.05	126.84	110.58
2	B	2340	NAP	O3X-P2B-O2X	5.21	127.22	107.38
2	B	2340	NAP	C3N-C7N-N7N	5.30	123.62	117.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1340	NAP	2	0
3	A	1342	MYC	2	0
2	B	2340	NAP	1	0
3	B	2342	MYC	4	0
2	C	3340	NAP	4	0
3	C	3342	MYC	2	0
2	D	4340	NAP	2	0
3	D	4342	MYC	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	320/337 (94%)	-0.16	2 (0%) 90 92	29, 45, 64, 79	0
1	B	326/337 (96%)	-0.25	1 (0%) 94 95	29, 44, 65, 88	0
1	C	325/337 (96%)	-0.33	0 100 100	27, 42, 62, 80	0
1	D	321/337 (95%)	-0.34	0 100 100	27, 41, 60, 80	0
All	All	1292/1348 (95%)	-0.27	3 (0%) 95 96	27, 43, 63, 88	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	269	GLU	2.2
1	A	178	ALA	2.1
1	B	88	MET	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(\AA^2)	Q<0.9
3	MYC	B	2342	23/23	0.92	0.17	1.44	44,55,56,57	0
3	MYC	A	1342	23/23	0.94	0.13	0.61	34,50,52,53	0
2	NAP	C	3340	48/48	0.98	0.10	0.09	24,32,46,51	0
3	MYC	A	1341	23/23	0.96	0.10	-0.10	36,40,41,42	0
2	NAP	B	2340	48/48	0.98	0.10	-0.18	29,35,51,55	0
3	MYC	B	2341	23/23	0.95	0.09	-0.27	36,41,42,43	0
2	NAP	A	1340	48/48	0.98	0.09	-0.31	30,35,53,59	0
2	NAP	D	4340	48/48	0.98	0.09	-0.36	22,31,48,53	0
3	MYC	C	3342	23/23	0.97	0.09	-0.50	26,30,33,33	0
3	MYC	D	4341	23/23	0.98	0.08	-0.69	28,31,32,33	0
3	MYC	D	4342	23/23	0.97	0.09	-0.97	28,31,33,34	0
3	MYC	C	3341	23/23	0.97	0.08	-1.21	29,31,32,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.