



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2018 – 01:17 PM EST

PDB ID : 5M67
Title : Crystal structure of S-adenosyl-L-homocysteine hydrolase from *Bradyrhizobium elkanii* in complex with adenine and 2'-deoxyadenosine
Authors : Manszewski, T.; Jaskolski, M.
Deposited on : 2016-10-24
Resolution : 1.54 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-20030736
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-20030736

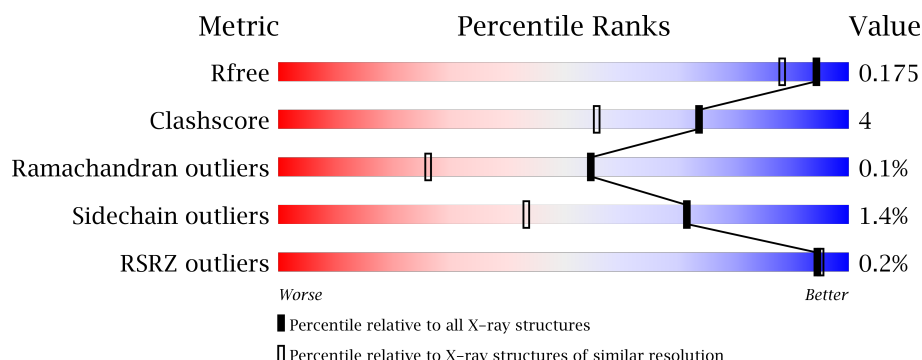
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.54 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	1773 (1.56-1.52)
Clashscore	112137	1845 (1.56-1.52)
Ramachandran outliers	110173	1810 (1.56-1.52)
Sidechain outliers	110143	1808 (1.56-1.52)
RSRZ outliers	101464	1774 (1.56-1.52)

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	479	<div> <div>90%</div> <div>7% ..</div> </div>
1	B	479	<div> <div>88%</div> <div>8% ..</div> </div>
1	C	479	<div> <div>91%</div> <div>6% ..</div> </div>
1	D	479	<div> <div>90%</div> <div>8% .</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PEG	A	505	-	-	X	X
5	PEG	B	504	-	-	-	X
5	PEG	D	504	-	-	X	X
6	ACT	B	505	-	-	-	X

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 17102 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 Adenosylhomocysteinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	468	Total	C	N	O	S	0	7	0
			3660	2320	630	687	23			
1	B	463	Total	C	N	O	S	0	11	0
			3645	2316	621	684	24			
1	C	468	Total	C	N	O	S	0	11	0
			3684	2336	633	692	23			
1	D	470	Total	C	N	O	S	0	9	0
			3691	2337	636	696	22			

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

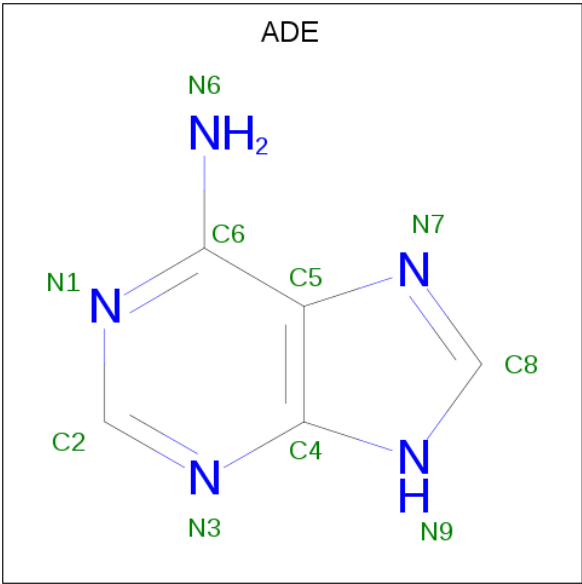
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Na	0	0
			1	1		
2	A	2	Total	Na	0	0
			2	2		
2	D	1	Total	Na	0	0
			1	1		
2	C	1	Total	Na	0	0
			1	1		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



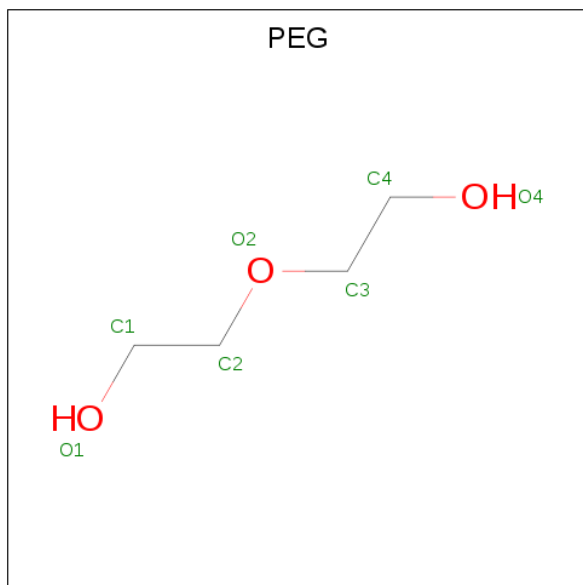
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is ADENINE (three-letter code: ADE) (formula: C₅H₅N₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			10	5	5		
4	B	1	Total	C	N	0	0
			10	5	5		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



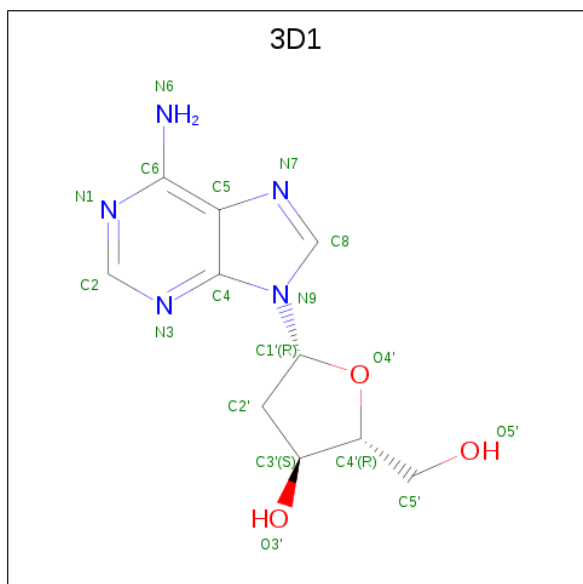
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 7 is (2R,3S,5R)-5-(6-amino-9H-purin-9-yl)-tetrahydro-2-(hydroxymethyl)furan-3-ol (three-letter code: 3D1) (formula: C₁₀H₁₃N₅O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	N	O	0	0
			18	10	5	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	D	1	Total	C	N	O	0	0
			18	10	5	3		

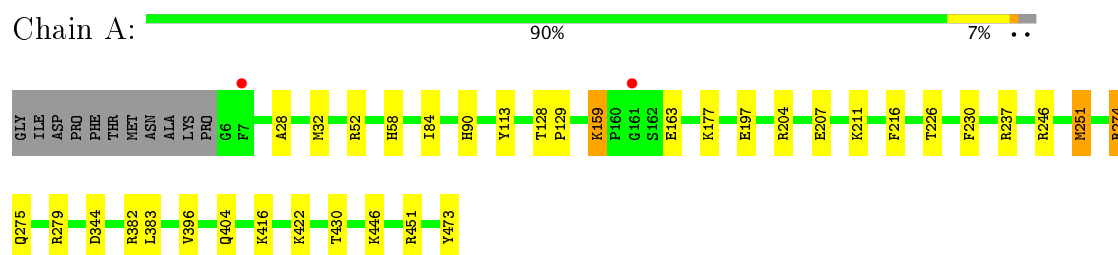
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	561	Total	O	0	0
			561	561		
8	B	580	Total	O	0	0
			580	580		
8	C	508	Total	O	0	0
			508	508		
8	D	507	Total	O	0	0
			507	507		

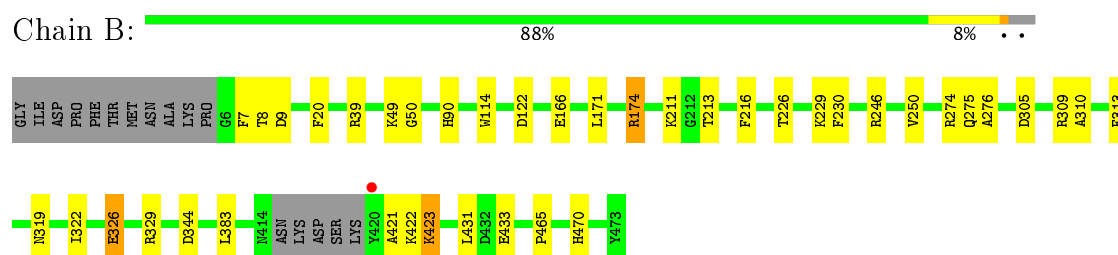
3 Residue-property plots

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

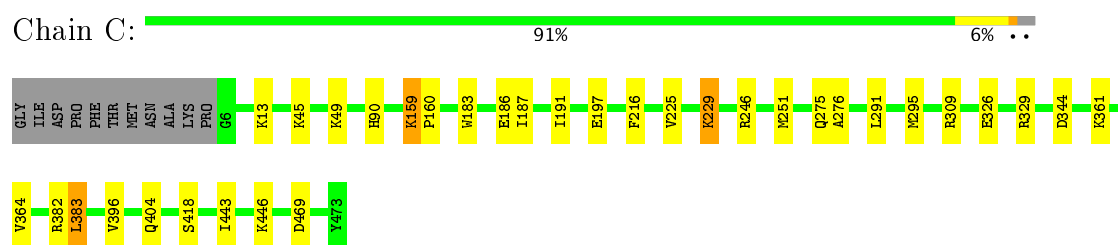
• Molecule 1: Adenosylhomocysteinase



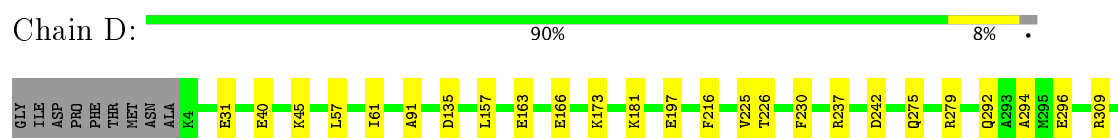
• Molecule 1: Adenosylhomocysteinase



• Molecule 1: Adenosylhomocysteinase



• Molecule 1: Adenosylhomocysteinase



I325	
H342	
F343	
D344	
K361	
D371	
K372	
H373	
R382	
L383	
K423	
K442	
K446	
E449	
D469	
R472	
Y473	

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	107.48 Å 174.53 Å 96.62 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.63 – 1.54 84.53 – 1.54	Depositor EDS
% Data completeness (in resolution range)	99.6 (43.63-1.54) 99.6 (84.53-1.54)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 1.53 Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, R_{free}	0.145 , 0.176 0.142 , 0.175	Depositor DCC
R_{free} test set	1015 reflections (0.38%)	DCC
Wilson B-factor (Å ²)	15.6	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	17102	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.09% 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, 0.333 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: 3D1, NAD, NA, ADE, ACT, PEG

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	0.75	0/3748	0.89	12/5056 (0.2%)
1	B	0.75	1/3747 (0.0%)	0.90	8/5055 (0.2%)
1	C	0.74	0/3781	0.83	5/5100 (0.1%)
1	D	0.74	0/3784	0.83	4/5106 (0.1%)
All	All	0.74	1/15060 (0.0%)	0.86	29/20317 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	326	GLU	CG-CD	5.34	1.59	1.51

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	309	ARG	NE-CZ-NH2	-8.97	115.81	120.30
1	A	52	ARG	NE-CZ-NH2	-8.28	116.16	120.30
1	D	309	ARG	NE-CZ-NH1	-8.06	116.27	120.30
1	B	246	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	A	274	ARG	NE-CZ-NH2	-7.98	116.31	120.30
1	B	39	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	B	246	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	A	451	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	A	204	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	A	451	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	B	174	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	B	309	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	C	383	LEU	CB-CG-CD2	-5.91	100.95	111.00
1	D	382[A]	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	D	382[B]	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	A	246	ARG	NE-CZ-NH2	-5.76	117.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	229[A]	LYS	CD-CE-NZ	5.71	124.83	111.70
1	C	229[B]	LYS	CD-CE-NZ	5.71	124.83	111.70
1	A	274	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	251[A]	MET	CG-SD-CE	-5.65	91.15	100.20
1	A	251[B]	MET	CG-SD-CE	-5.65	91.15	100.20
1	C	309	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	C	246	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	A	204	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	B	250	VAL	CG1-CB-CG2	5.26	119.31	110.90
1	A	383	LEU	CB-CG-CD1	-5.18	102.20	111.00
1	B	344	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	52	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	D	242	ASP	CB-CG-OD2	-5.01	113.79	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	3660	0	3695	25	0
1	B	3645	0	3688	26	0
1	C	3684	0	3725	25	0
1	D	3691	0	3715	33	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	44	0	26	1	0
3	B	44	0	26	1	0
3	C	44	0	26	2	0
3	D	44	0	26	2	0
4	A	10	0	4	1	0
4	B	10	0	4	0	0
5	A	7	0	9	10	0
5	B	7	0	9	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	7	0	9	9	0
6	B	4	0	3	0	0
6	C	4	0	3	0	0
7	C	18	0	13	3	0
7	D	18	0	13	4	0
8	A	561	0	0	10	0
8	B	580	0	0	8	0
8	C	508	0	0	7	0
8	D	507	0	0	15	0
All	All	17102	0	14994	114	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 (114) 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:344[A]:ASP:O	8:D:601:HOH:O	1.64	1.15
1:D:344[B]:ASP:O	8:D:602:HOH:O	1.74	1.03
1:C:344[A]:ASP:O	8:C:602:HOH:O	1.82	0.97
1:C:382[B]:ARG:NH2	8:C:603:HOH:O	1.99	0.94
5:A:505:PEG:H41	8:A:970:HOH:O	1.69	0.93
1:B:305[B]:ASP:OD2	8:B:601:HOH:O	1.91	0.88
5:D:504:PEG:H12	8:D:990:HOH:O	1.75	0.86
1:C:159:LYS:HD3	1:C:160:PRO:HD2	1.56	0.85
5:A:505:PEG:H31	1:C:275:GLN:O	1.77	0.83
1:C:326:GLU:OE1	1:C:329:ARG:NH1	2.12	0.81
1:A:237:ARG:HG2	5:A:505:PEG:H11	1.64	0.79
1:A:237:ARG:CZ	5:A:505:PEG:H42	2.13	0.77
1:D:237:ARG:HG2	5:D:504:PEG:H42	1.66	0.76
7:D:503:3D1:H2'2	8:D:609:HOH:O	1.83	0.76
1:B:122[A]:ASP:OD1	8:B:602:HOH:O	2.05	0.74
1:B:275:GLN:O	5:D:504:PEG:H22	1.87	0.73
7:C:503:3D1:H2'2	8:C:609:HOH:O	1.88	0.73
1:D:449[B]:GLU:OE1	8:D:604:HOH:O	2.06	0.72
1:C:469[B]:ASP:OD2	8:C:604:HOH:O	2.10	0.69
1:D:31:GLU:OE2	1:D:442:LYS:NZ	2.24	0.69
1:B:166[A]:GLU:OE1	8:B:603:HOH:O	2.13	0.66
4:A:504:ADE:N9	8:A:604:HOH:O	2.29	0.65
1:A:446:LYS:HD2	8:A:936:HOH:O	1.97	0.64
1:B:470:HIS:HD2	8:B:852:HOH:O	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:505:PEG:H22	1:C:276:ALA:HA	1.81	0.61
1:B:211:LYS:HG3	1:B:213:THR:HG23	1.82	0.61
1:B:274[B]:ARG:HD2	8:B:854:HOH:O	2.01	0.61
5:A:505:PEG:H12	8:A:812:HOH:O	2.02	0.60
1:B:383[B]:LEU:HD22	3:B:502:NAD:N7N	2.16	0.60
1:D:446:LYS:HG2	8:D:711:HOH:O	2.02	0.59
1:A:237:ARG:NE	5:A:505:PEG:H42	2.17	0.59
1:C:229[A]:LYS:HE3	1:D:472:ARG:HB2	1.85	0.58
1:C:469[B]:ASP:CG	8:C:604:HOH:O	2.42	0.58
1:D:237:ARG:HG2	5:D:504:PEG:C4	2.34	0.57
1:B:275:GLN:O	5:D:504:PEG:H31	2.05	0.57
1:D:163:GLU:O	1:D:166:GLU:HG3	2.04	0.56
1:C:159:LYS:HD3	1:C:160:PRO:CD	2.34	0.55
1:D:342:HIS:HA	1:D:383:LEU:HD21	1.87	0.55
1:A:275:GLN:CB	5:A:505:PEG:H21	2.36	0.55
1:B:326:GLU:HG3	8:B:618:HOH:O	2.07	0.55
1:B:20:PHE:HB2	5:B:504:PEG:H11	1.89	0.54
1:C:344[A]:ASP:HB3	1:C:382[A]:ARG:HG2	1.89	0.53
1:D:279[B]:ARG:HD2	8:D:603:HOH:O	2.06	0.53
1:B:20:PHE:CG	5:B:504:PEG:H32	2.44	0.53
1:D:237:ARG:CZ	5:D:504:PEG:H11	2.38	0.53
1:A:275:GLN:HB2	5:A:505:PEG:H21	1.91	0.52
1:C:13:LYS:HE2	8:C:1006:HOH:O	2.09	0.52
1:B:174:ARG:NE	8:B:606:HOH:O	2.23	0.51
1:A:446:LYS:HB3	8:A:997:HOH:O	2.12	0.50
5:B:504:PEG:H31	1:D:361:LYS:HA	1.93	0.50
1:B:49:LYS:HD3	1:B:50:GLY:N	2.26	0.50
1:B:423:LYS:HE3	1:B:423:LYS:HA	1.94	0.49
1:B:7:PHE:CE1	1:B:9:ASP:HB3	2.46	0.49
1:D:449[A]:GLU:HG2	8:D:618:HOH:O	2.13	0.49
7:D:503:3D1:H1'	8:D:621:HOH:O	2.13	0.49
3:D:502:NAD:C4N	7:D:503:3D1:H3'	2.43	0.48
5:A:505:PEG:H22	1:C:275:GLN:O	2.13	0.48
1:A:473:TYR:O	1:B:229:LYS:HE2	2.14	0.48
3:C:502:NAD:C4N	7:C:503:3D1:H3'	2.44	0.48
1:D:279[B]:ARG:NH1	8:D:603:HOH:O	1.96	0.48
1:D:275:GLN:HG3	5:D:504:PEG:H32	1.96	0.47
1:A:251[A]:MET:HE1	1:C:396:VAL:HB	1.95	0.47
1:D:57:LEU:HD21	8:D:621:HOH:O	2.14	0.47
1:C:197:GLU:HB2	1:C:404:GLN:HE21	1.80	0.47
1:A:430:THR:HG23	8:A:963:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:503:3D1:C2'	8:C:609:HOH:O	2.54	0.47
1:C:361:LYS:HE2	1:C:364:VAL:HG21	1.97	0.46
1:C:443:ILE:HD12	1:D:294:ALA:HB1	1.97	0.46
1:D:135:ASP:OD2	1:D:197:GLU:HG2	2.15	0.46
1:A:344:ASP:HB3	1:A:382[A]:ARG:HG2	1.98	0.46
1:B:319:ASN:HB3	1:B:322:ILE:HD11	1.97	0.46
1:C:225:VAL:HG22	1:D:472:ARG:CZ	2.45	0.46
1:D:423:LYS:HB2	8:D:907:HOH:O	2.16	0.46
7:D:503:3D1:C2'	8:D:609:HOH:O	2.54	0.46
1:A:84:ILE:HG22	1:A:113:TYR:HB2	1.97	0.46
1:A:251[A]:MET:CE	1:C:396:VAL:HB	2.46	0.45
1:D:371:ASP:OD1	1:D:373:HIS:HB3	2.15	0.45
1:D:442:LYS:HE3	8:D:1028:HOH:O	2.18	0.44
1:A:128:THR:HB	1:A:129:PRO:HD2	1.99	0.44
1:A:382[A]:ARG:NH2	8:A:624:HOH:O	2.50	0.44
1:B:433:GLU:OE1	1:B:465:PRO:HA	2.18	0.44
1:B:226:THR:HA	1:B:230:PHE:CD1	2.53	0.43
1:B:329:ARG:HD2	8:B:618:HOH:O	2.17	0.43
1:B:114:TRP:HB3	1:B:171:LEU:HD22	2.00	0.43
1:D:446:LYS:HD3	8:D:705:HOH:O	2.17	0.43
1:D:292:GLN:O	1:D:296:GLU:HG2	2.19	0.43
1:A:226:THR:HA	1:A:230:PHE:CD1	2.53	0.43
1:A:177:LYS:HB2	1:A:177:LYS:NZ	2.34	0.42
1:A:128:THR:HB	1:A:129:PRO:CD	2.49	0.42
1:D:225:VAL:HG21	1:D:473:TYR:CE1	2.54	0.42
1:A:396:VAL:HB	1:C:251[A]:MET:CE	2.49	0.42
1:C:291:LEU:O	1:C:295[A]:MET:HG2	2.20	0.41
1:A:159:LYS:HA	1:A:159:LYS:NZ	2.35	0.41
1:C:383:LEU:HD22	3:C:502:NAD:N7N	2.35	0.41
3:A:503:NAD:H8A	8:A:829:HOH:O	2.19	0.41
1:B:276:ALA:HA	5:D:504:PEG:H31	2.01	0.41
1:A:197:GLU:HB2	1:A:404:GLN:HE21	1.86	0.41
1:D:157:LEU:HB3	1:D:173:LYS:HE3	2.03	0.41
1:D:275:GLN:CB	5:D:504:PEG:H32	2.51	0.41
1:D:383:LEU:HD22	3:D:502:NAD:N7N	2.35	0.41
1:A:207:GLU:O	1:A:211:LYS:HG3	2.21	0.41
1:D:325:ILE:HD12	1:D:325:ILE:HA	1.84	0.41
1:A:274:ARG:HD2	8:A:821:HOH:O	2.20	0.41
1:A:279[A]:ARG:NH1	8:A:615:HOH:O	2.43	0.41
1:B:310:ALA:HB3	1:B:313:PHE:CZ	2.56	0.41
1:D:61:ILE:HD13	1:D:91:ALA:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:423:LYS:HB3	1:D:423:LYS:HE2	1.90	0.40
1:A:28:ALA:O	1:A:32:MET:HG3	2.21	0.40
1:C:187:ILE:O	1:C:191:ILE:HG12	2.21	0.40
1:C:49:LYS:HE3	1:C:49:LYS:HB2	1.86	0.40
1:C:183:TRP:O	1:C:186:GLU:HB3	2.21	0.40
1:B:431:LEU:HA	1:B:431:LEU:HD23	1.90	0.40
1:D:226:THR:HA	1:D:230:PHE:CD1	2.56	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	473/479 (99%)	461 (98%)	11 (2%)	1 (0%)	51	24
1	B	471/479 (98%)	458 (97%)	12 (2%)	1 (0%)	51	24
1	C	477/479 (100%)	463 (97%)	14 (3%)	0	100	100
1	D	477/479 (100%)	467 (98%)	10 (2%)	0	100	100
All	All	1898/1916 (99%)	1849 (97%)	47 (2%)	2 (0%)	55	26

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	421	ALA
1	A	58	HIS

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	385/387 (100%)	379 (98%)	6 (2%)	68	37
1	B	385/387 (100%)	381 (99%)	4 (1%)	80	59
1	C	389/387 (100%)	383 (98%)	6 (2%)	70	40
1	D	389/387 (100%)	383 (98%)	6 (2%)	70	40
All	All	1548/1548 (100%)	1526 (99%)	22 (1%)	71	43

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	HIS
1	A	159	LYS
1	A	163	GLU
1	A	216	PHE
1	A	416	LYS
1	A	422	LYS
1	B	90	HIS
1	B	216	PHE
1	B	422	LYS
1	B	423	LYS
1	C	45	LYS
1	C	90	HIS
1	C	159	LYS
1	C	216	PHE
1	C	418	SER
1	C	446	LYS
1	D	40	GLU
1	D	45	LYS
1	D	181	LYS
1	D	216	PHE
1	D	469[A]	ASP
1	D	469[B]	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 5 are monoatomic - leaving 13 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	NAD	A	503	-	41,48,48	1.86	9 (21%)	43,73,73	1.80	7 (16%)
4	ADE	A	504	-	9,11,11	0.63	0	7,15,15	0.90	0
5	PEG	A	505	-	6,6,6	0.81	0	5,5,5	1.00	0
3	NAD	B	502	-	41,48,48	1.67	12 (29%)	43,73,73	1.94	6 (13%)
4	ADE	B	503	-	9,11,11	1.18	2 (22%)	7,15,15	0.94	0
5	PEG	B	504	-	6,6,6	0.66	0	5,5,5	0.70	0
6	ACT	B	505	-	1,3,3	2.96	1 (100%)	0,3,3	0.00	-
3	NAD	C	502	-	41,48,48	1.68	9 (21%)	43,73,73	2.06	6 (13%)
7	3D1	C	503	-	17,20,20	1.51	3 (17%)	18,29,29	2.64	5 (27%)
6	ACT	C	504	-	1,3,3	3.20	1 (100%)	0,3,3	0.00	-
3	NAD	D	502	-	41,48,48	1.93	10 (24%)	43,73,73	1.88	6 (13%)
7	3D1	D	503	-	17,20,20	1.26	1 (5%)	18,29,29	2.39	7 (38%)
5	PEG	D	504	-	6,6,6	0.72	0	5,5,5	1.47	1 (20%)

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	NAD	A	503	-	-	0/22/62/62	0/5/5/5
4	ADE	A	504	-	-	0/0/0/0	0/2/2/2
5	PEG	A	505	-	-	0/4/4/4	0/0/0/0
3	NAD	B	502	-	-	0/22/62/62	0/5/5/5
4	ADE	B	503	-	-	0/0/0/0	0/2/2/2
5	PEG	B	504	-	-	0/4/4/4	0/0/0/0
6	ACT	B	505	-	-	0/0/0/0	0/0/0/0
3	NAD	C	502	-	-	0/22/62/62	0/5/5/5
7	3D1	C	503	-	-	0/2/18/18	0/3/3/3
6	ACT	C	504	-	-	0/0/0/0	0/0/0/0
3	NAD	D	502	-	-	0/22/62/62	0/5/5/5
7	3D1	D	503	-	-	0/2/18/18	0/3/3/3
5	PEG	D	504	-	-	0/4/4/4	0/0/0/0

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	503	NAD	C2B-C3B	-4.11	1.42	1.53
3	A	503	NAD	C2B-C1B	-4.07	1.47	1.53
3	C	502	NAD	C2B-C1B	-3.83	1.47	1.53
3	D	502	NAD	C2B-C1B	-3.66	1.47	1.53
3	D	502	NAD	C2B-C3B	-3.56	1.44	1.53
3	C	502	NAD	C2B-C3B	-3.41	1.44	1.53
3	B	502	NAD	C2B-C3B	-3.30	1.44	1.53
3	C	502	NAD	O4B-C4B	-2.69	1.38	1.45
3	D	502	NAD	O4B-C4B	-2.24	1.39	1.45
3	A	503	NAD	C2D-C1D	-2.24	1.50	1.53
4	B	503	ADE	C4-N3	-2.20	1.33	1.37
3	B	502	NAD	O4B-C4B	-2.14	1.40	1.45
3	B	502	NAD	C2B-C1B	-2.10	1.50	1.53
4	B	503	ADE	C2-N3	2.11	1.35	1.32
7	C	503	3D1	C6-N6	2.11	1.42	1.34
7	C	503	3D1	O3'-C3'	2.12	1.48	1.43
3	B	502	NAD	C4A-N3A	2.12	1.38	1.35
7	D	503	3D1	C2-N1	2.15	1.37	1.33
3	B	502	NAD	C6N-C5N	2.16	1.43	1.38
3	C	502	NAD	C2A-N1A	2.19	1.38	1.33
3	B	502	NAD	C6N-N1N	2.36	1.41	1.35
3	B	502	NAD	C7N-N7N	2.39	1.37	1.33
3	D	502	NAD	C2A-N1A	2.46	1.38	1.33
3	D	502	NAD	O4D-C1D	2.47	1.44	1.41
3	B	502	NAD	C6A-N6A	2.48	1.44	1.34
3	A	503	NAD	C6A-N6A	2.53	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	NAD	C2A-N1A	2.68	1.38	1.33
3	D	502	NAD	C6A-N6A	2.71	1.45	1.34
3	A	503	NAD	C8A-N7A	2.74	1.39	1.34
3	C	502	NAD	O2B-C2B	2.75	1.49	1.43
7	C	503	3D1	C4-N3	2.75	1.39	1.35
3	A	503	NAD	C6N-N1N	2.78	1.42	1.35
3	B	502	NAD	O4D-C1D	2.84	1.45	1.41
6	B	505	ACT	CH3-C	2.96	1.52	1.48
3	D	502	NAD	C6N-N1N	2.97	1.43	1.35
3	A	503	NAD	C5N-C4N	3.05	1.44	1.38
3	C	502	NAD	C6A-N6A	3.07	1.46	1.34
3	C	502	NAD	C4N-C3N	3.09	1.44	1.39
6	C	504	ACT	CH3-C	3.20	1.52	1.48
3	C	502	NAD	C7N-N7N	3.29	1.39	1.33
3	B	502	NAD	C4N-C3N	3.76	1.45	1.39
3	D	502	NAD	C5N-C4N	4.07	1.46	1.38
3	A	503	NAD	C4N-C3N	4.28	1.46	1.39
3	B	502	NAD	C5N-C4N	4.33	1.47	1.38
3	C	502	NAD	C5N-C4N	4.46	1.47	1.38
3	D	502	NAD	C4N-C3N	4.79	1.47	1.39
3	A	503	NAD	C7N-N7N	5.11	1.43	1.33
3	D	502	NAD	C7N-N7N	5.15	1.43	1.33

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	502	NAD	N3A-C2A-N1A	-8.69	121.29	128.86
3	C	502	NAD	N3A-C2A-N1A	-8.18	121.74	128.86
7	C	503	3D1	N3-C2-N1	-7.64	122.20	128.86
3	A	503	NAD	N3A-C2A-N1A	-7.63	122.21	128.86
3	B	502	NAD	N3A-C2A-N1A	-6.85	122.89	128.86
3	C	502	NAD	C4B-O4B-C1B	-5.90	103.48	109.77
3	B	502	NAD	C5N-C4N-C3N	-5.62	113.75	120.35
3	C	502	NAD	C4A-C5A-N7A	-5.08	104.50	109.41
7	D	503	3D1	O4'-C1'-C2'	-4.79	97.07	106.25
3	A	503	NAD	C4B-O4B-C1B	-4.56	104.92	109.77
3	C	502	NAD	C5N-C4N-C3N	-4.52	115.03	120.35
7	D	503	3D1	C4-C5-N7	-4.35	105.21	109.41
3	B	502	NAD	C4A-C5A-N7A	-4.21	105.34	109.41
3	D	502	NAD	C5N-C4N-C3N	-4.19	115.42	120.35
3	B	502	NAD	C4B-O4B-C1B	-4.13	105.37	109.77
7	D	503	3D1	N3-C2-N1	-3.44	125.86	128.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	503	3D1	O5'-C5'-C4'	-3.43	99.81	111.34
7	C	503	3D1	O4'-C1'-C2'	-3.17	100.17	106.25
7	D	503	3D1	C2'-C1'-N9	-3.03	107.07	114.23
3	A	503	NAD	C4D-O4D-C1D	-2.66	106.93	109.77
3	A	503	NAD	C4A-C5A-N7A	-2.61	106.89	109.41
3	A	503	NAD	C3N-C2N-N1N	-2.57	117.84	120.43
7	C	503	3D1	O5'-C5'-C4'	-2.47	103.04	111.34
7	C	503	3D1	C2'-C1'-N9	-2.35	108.69	114.23
7	D	503	3D1	C5'-C4'-C3'	-2.19	109.28	114.84
3	D	502	NAD	C4D-O4D-C1D	-2.12	107.51	109.77
3	A	503	NAD	O7N-C7N-N7N	-2.10	119.59	122.58
3	D	502	NAD	C4B-O4B-C1B	-2.01	107.63	109.77
3	C	502	NAD	O4B-C4B-C3B	2.02	109.18	105.17
3	D	502	NAD	C5N-C6N-N1N	2.19	123.78	120.40
3	B	502	NAD	C3N-C7N-N7N	2.23	120.32	117.77
5	D	504	PEG	C3-O2-C2	2.66	124.80	113.30
3	D	502	NAD	C2N-C3N-C4N	3.11	121.81	118.26
3	C	502	NAD	C2N-C3N-C4N	3.18	121.89	118.26
3	A	503	NAD	C2N-C3N-C4N	3.19	121.90	118.26
7	D	503	3D1	O4'-C1'-N9	3.64	113.92	107.78
3	B	502	NAD	C2N-C3N-C4N	3.64	122.42	118.26
7	C	503	3D1	O4'-C1'-N9	5.35	116.79	107.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	NAD	1	0
4	A	504	ADE	1	0
5	A	505	PEG	10	0
3	B	502	NAD	1	0
5	B	504	PEG	3	0
3	C	502	NAD	2	0
7	C	503	3D1	3	0
3	D	502	NAD	2	0
7	D	503	3D1	4	0
5	D	504	PEG	9	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [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	468/479 (97%)	-0.76	2 (0%) 92 93	11, 18, 40, 66	1 (0%)
1	B	463/479 (96%)	-0.76	1 (0%) 94 95	11, 17, 37, 68	1 (0%)
1	C	468/479 (97%)	-0.73	0 100 100	11, 20, 43, 86	0
1	D	470/479 (98%)	-0.66	0 100 100	11, 20, 42, 70	0
All	All	1869/1916 (97%)	-0.73	3 (0%) 94 95	11, 19, 40, 86	2 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	420	TYR	2.8
1	A	161	GLY	2.7
1	A	7	PHE	2.1

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
5	PEG	D	504	7/7	0.91	0.24	23.83	14,18,20,36	7
5	PEG	B	504	7/7	0.80	0.21	16.68	45,50,55,56	0
5	PEG	A	505	7/7	0.90	0.20	13.51	15,18,24,27	7
6	ACT	B	505	4/4	0.89	0.13	4.13	31,32,35,37	0
6	ACT	C	504	4/4	0.94	0.14	1.87	27,35,36,37	0
7	3D1	C	503	18/18	0.97	0.06	0.53	12,15,27,30	0
7	3D1	D	503	18/18	0.97	0.07	0.41	11,14,26,29	0
3	NAD	A	503	44/44	0.98	0.06	-0.01	12,15,17,19	0
4	ADE	A	504	10/10	0.99	0.05	-0.10	10,11,12,13	0
3	NAD	D	502	44/44	0.98	0.06	-0.16	10,14,19,19	0
3	NAD	C	502	44/44	0.98	0.05	-0.20	10,15,18,20	0
4	ADE	B	503	10/10	0.98	0.04	-0.26	11,11,13,14	0
2	NA	B	501	1/1	1.00	0.04	-0.31	13,13,13,13	0
2	NA	A	501	1/1	1.00	0.04	-0.60	13,13,13,13	0
3	NAD	B	502	44/44	0.98	0.05	-0.66	12,15,18,18	0
2	NA	D	501	1/1	1.00	0.03	-1.87	14,14,14,14	0
2	NA	C	501	1/1	1.00	0.04	-2.75	14,14,14,14	0
2	NA	A	502	1/1	0.99	0.07	-	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.