



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:35 PM UTC

PDB ID : 6D8P / pdb_00006d8p
Title : Ternary RsAgo Complex Containing Guide RNA Paired with Target DNA
Authors : Liu, Y.; Esyunina, D.; Olovnikov, I.; Teplova, M.; Patel, D.J.
Deposited on : 2018-04-26
Resolution : 2.10 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
3	G	24	 71% 12% 17%
3	J	24	 67% 12% 21%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14004 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	758	Total	C	N	O	S	0	5	0
			5918	3755	1067	1080	16			
1	B	752	Total	C	N	O	S	0	2	0
			5685	3630	992	1047	16			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP A4WYU7
A	-12	HIS	-	expression tag	UNP A4WYU7
A	-11	HIS	-	expression tag	UNP A4WYU7
A	-10	HIS	-	expression tag	UNP A4WYU7
A	-9	HIS	-	expression tag	UNP A4WYU7
A	-8	HIS	-	expression tag	UNP A4WYU7
A	-7	HIS	-	expression tag	UNP A4WYU7
A	-6	ASP	-	expression tag	UNP A4WYU7
A	-5	TYR	-	expression tag	UNP A4WYU7
A	-4	LYS	-	expression tag	UNP A4WYU7
A	-3	ASP	-	expression tag	UNP A4WYU7
A	-2	ASP	-	expression tag	UNP A4WYU7
A	-1	ASP	-	expression tag	UNP A4WYU7
A	0	ASP	-	expression tag	UNP A4WYU7
A	1	LYS	-	expression tag	UNP A4WYU7
B	-13	MET	-	initiating methionine	UNP A4WYU7
B	-12	HIS	-	expression tag	UNP A4WYU7
B	-11	HIS	-	expression tag	UNP A4WYU7
B	-10	HIS	-	expression tag	UNP A4WYU7
B	-9	HIS	-	expression tag	UNP A4WYU7
B	-8	HIS	-	expression tag	UNP A4WYU7
B	-7	HIS	-	expression tag	UNP A4WYU7
B	-6	ASP	-	expression tag	UNP A4WYU7
B	-5	TYR	-	expression tag	UNP A4WYU7
B	-4	LYS	-	expression tag	UNP A4WYU7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	ASP	-	expression tag	UNP A4WYU7
B	-2	ASP	-	expression tag	UNP A4WYU7
B	-1	ASP	-	expression tag	UNP A4WYU7
B	0	ASP	-	expression tag	UNP A4WYU7
B	1	LYS	-	expression tag	UNP A4WYU7

- Molecule 2 is a RNA chain called RNA (5'-R(P*UP*UP*AP*CP*UP*GP*CP*AP*CP*AP*GP*GP*UP*GP*AP*CP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	18	Total	C	N	O	P	0	0	0
			386	172	70	126	18			
2	C	18	Total	C	N	O	P	0	0	0
			386	172	70	126	18			

- Molecule 3 is a DNA chain called DNA (5'-D(P*TP*CP*GP*TP*CP*AP*CP*CP*TP*GP*TP*GP*CP*AP*GP*TP*AP*AP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	19	Total	C	N	O	P	0	0	0
			386	184	68	115	19			
3	G	20	Total	C	N	O	P	0	0	0
			408	194	73	121	20			

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	Mg	0	0
			5	5		
4	E	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



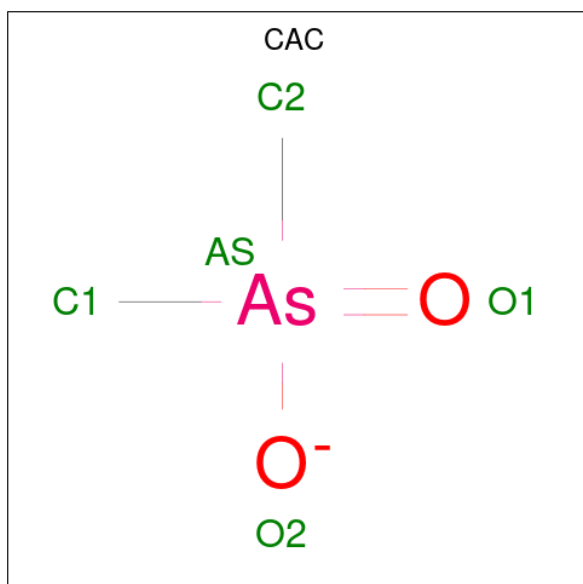
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total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

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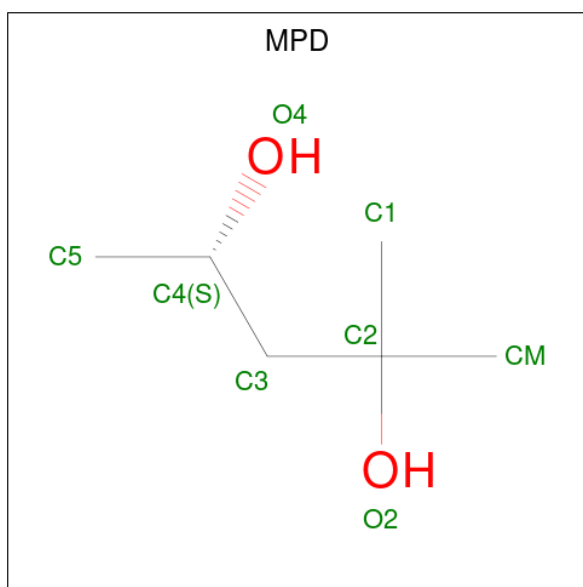
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	J	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	G	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is CACODYLATE ION (CCD ID: CAC) (formula: $C_2H_6AsO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total 5	As 1	C 2	O 2	0	0
6	A	1	Total 5	As 1	C 2	O 2	0	0
6	A	1	Total 5	As 1	C 2	O 2	0	0
6	B	1	Total 5	As 1	C 2	O 2	0	0

- Molecule 7 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C O 8 6 2	0	0

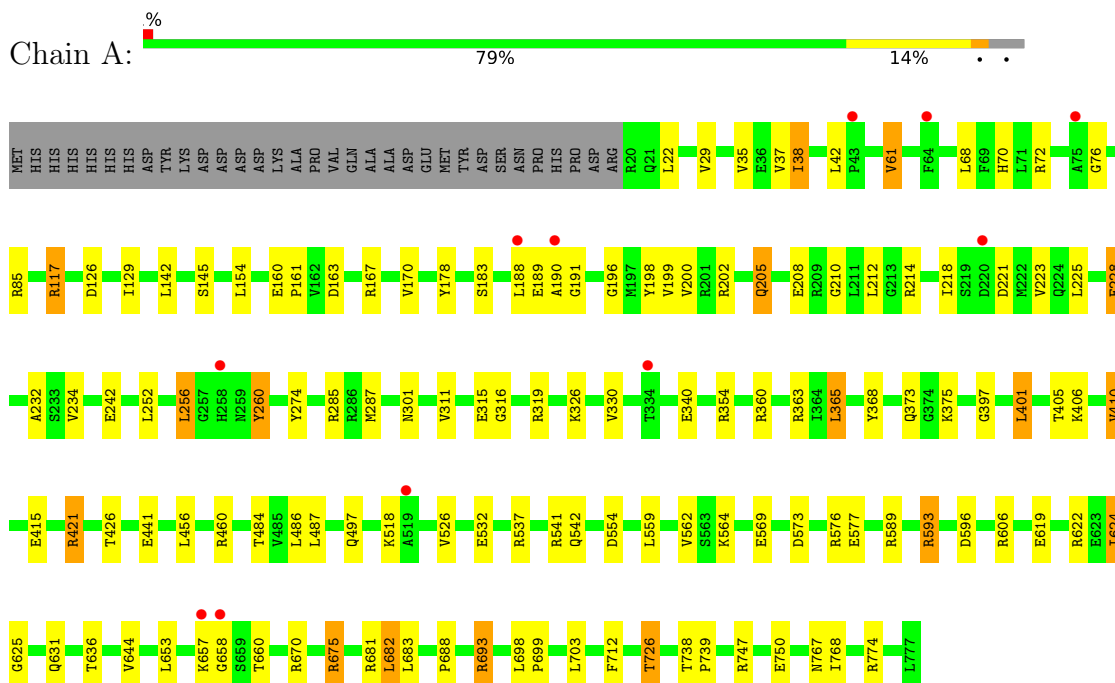
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	354	Total O 354 354	0	0
8	E	52	Total O 52 52	0	0
8	J	38	Total O 38 38	0	0
8	B	217	Total O 217 217	0	0
8	C	34	Total O 34 34	0	0
8	G	25	Total O 25 25	0	0

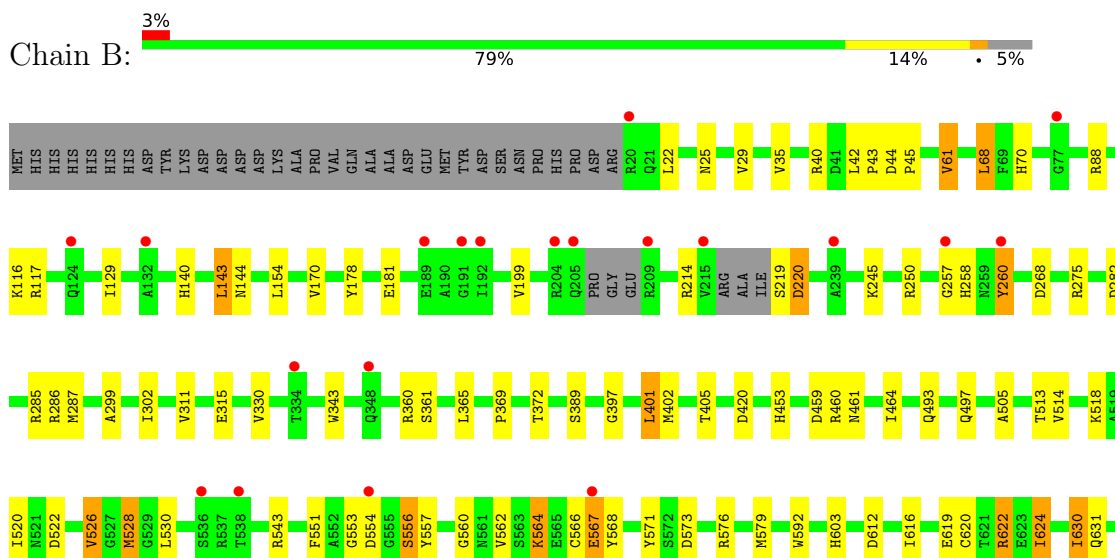
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Uncharacterized protein



- Molecule 1: Uncharacterized protein

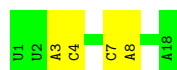
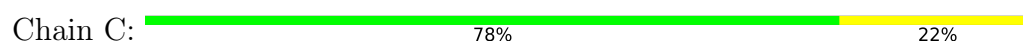




- Molecule 2: RNA (5'-R(P*UP*UP*AP*CP*UP*GP*CP*AP*CP*AP*GP*GP*UP*GP*AP*CP*GP*A)-3')



- Molecule 2: RNA (5'-R(P*UP*UP*AP*CP*UP*GP*CP*AP*CP*AP*GP*GP*UP*GP*AP*CP*GP*A)-3')



- Molecule 3: DNA (5'-D(P*TP*CP*GP*TP*CP*AP*CP*CP*TP*GP*TP*GP*CP*AP*GP*T*P*AP*AP*C)-3')



- Molecule 3: DNA (5'-D(P*TP*CP*GP*TP*CP*AP*CP*CP*TP*GP*TP*GP*CP*AP*GP*T*P*AP*AP*C)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.23Å 119.22Å 117.65Å 90.00° 95.62° 90.00°	Depositor
Resolution (Å)	42.34 – 2.10 42.34 – 2.10	Depositor EDS
% Data completeness (in resolution range)	93.4 (42.34-2.10) 89.3 (42.34-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.182 , 0.235 (Not available) , 0.226	Depositor DCC
R_{free} test set	5085 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å ²)	35.3	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14004	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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: ACT, MPD, CAC, MG

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	0.52	0/6059	0.84	0/8223
1	B	0.48	0/5817	0.84	4/7920 (0.1%)
2	C	0.29	0/431	0.51	0/668
2	E	0.31	0/431	0.51	0/668
3	G	0.29	0/456	0.98	0/701
3	J	0.31	0/431	0.93	0/662
All	All	0.48	0/13625	0.83	4/18842 (0.0%)

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	B	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	44	ASP	CA-C-N	6.90	126.87	119.28
1	B	44	ASP	C-N-CA	6.90	126.87	119.28
1	B	567	GLU	N-CA-C	6.78	125.25	110.80
1	B	676	VAL	N-CA-C	-5.43	107.14	111.81

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	566	CYS	Peptide

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	5918	0	5850	64	0
1	B	5685	0	5462	67	0
2	C	386	0	195	2	0
2	E	386	0	195	5	0
3	G	408	0	226	3	0
3	J	386	0	215	3	0
4	A	5	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
5	A	48	0	36	1	0
5	B	16	0	12	0	0
5	E	8	0	6	0	0
5	G	4	0	3	1	0
5	J	4	0	3	0	0
6	A	15	0	0	0	0
6	B	5	0	0	0	0
7	C	8	0	14	1	0
8	A	354	0	0	5	0
8	B	217	0	0	5	0
8	C	34	0	0	0	0
8	E	52	0	0	1	0
8	G	25	0	0	0	0
8	J	38	0	0	0	0
All	All	14004	0	12217	140	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 (140) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:576[B]:ARG:HD2	1:A:619:GLU:HG3	1.59	0.83
1:B:258:HIS:HA	1:B:260:TYR:H	1.44	0.83
1:A:421:ARG:HG2	1:A:456:LEU:HD21	1.64	0.78
1:B:88:ARG:NH1	8:B:902:HOH:O	2.16	0.78
1:B:268:ASP:OD2	1:B:693:ARG:NH2	2.18	0.77
1:B:603:HIS:ND1	1:B:741:THR:HG21	2.02	0.75
1:B:282:ASP:OD1	1:B:285:ARG:NH1	2.18	0.75
1:B:726:THR:OG1	1:B:736:ALA:O	2.09	0.70
1:B:61:VAL:HG13	1:B:68:LEU:HD21	1.74	0.70
1:A:365:LEU:HD23	1:A:410:VAL:HG22	1.72	0.70
1:B:528:MET:HE1	1:B:571:TYR:HB2	1.75	0.68
1:B:573:ASP:OD1	1:B:576:ARG:NH2	2.27	0.67
1:A:693:ARG:HG2	3:J:2:DT:H5'	1.78	0.66
1:B:178:TYR:O	8:B:901:HOH:O	2.13	0.66
1:A:576[B]:ARG:NH1	1:A:577:GLU:OE2	2.29	0.65
1:B:543:ARG:NH2	1:B:568:TYR:OH	2.29	0.65
1:A:360:ARG:HB3	1:A:405:THR:HG23	1.80	0.64
1:A:117:ARG:NH2	8:A:905:HOH:O	2.32	0.63
1:B:513:THR:HG23	1:B:557:TYR:O	1.98	0.63
1:A:573:ASP:OD1	1:A:576[A]:ARG:NH2	2.32	0.63
1:A:154:LEU:HD11	1:A:287:MET:HE2	1.81	0.62
1:A:698:LEU:HD12	1:A:699:PRO:HD2	1.83	0.61
1:B:401:LEU:HD13	1:B:402:MET:HE2	1.82	0.61
1:B:154:LEU:HD21	1:B:287:MET:HE2	1.83	0.60
1:B:723:LEU:O	1:B:726:THR:HG22	2.00	0.60
1:B:360:ARG:HB3	1:B:405:THR:HG23	1.84	0.60
1:A:242:GLU:OE1	1:A:537:ARG:NH2	2.35	0.59
1:A:198:TYR:CZ	1:A:214:ARG:HD2	2.37	0.59
1:B:553:GLY:N	1:B:556:SER:O	2.27	0.59
1:A:161:PRO:HG3	1:A:167:ARG:HD2	1.85	0.58
1:B:40:ARG:HG2	1:B:70:HIS:HE1	1.67	0.58
1:B:513:THR:HG21	1:B:556:SER:HB3	1.85	0.58
1:A:670:ARG:HH22	1:A:726:THR:CG2	2.17	0.57
3:G:-5:DT:H3'	5:G:101:ACT:H2	1.86	0.57
2:C:3:A:H2'	2:C:4:C:C6	2.39	0.57
2:E:3:A:H2'	2:E:4:C:C6	2.40	0.56
3:J:5:DC:C6	3:J:5:DC:H5'	2.41	0.56
1:B:513:THR:HG22	1:B:514:VAL:N	2.21	0.55
1:B:315:GLU:O	8:B:903:HOH:O	2.18	0.55
1:B:219:SER:OG	1:B:220:ASP:N	2.39	0.55
1:B:670:ARG:HH22	1:B:726:THR:CG2	2.20	0.55
1:A:38:ILE:HG22	1:A:70:HIS:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:ARG:NH1	1:A:441:GLU:O	2.40	0.54
1:A:670:ARG:HH22	1:A:726:THR:HG22	1.71	0.54
1:B:576:ARG:HD3	1:B:616:ILE:HD13	1.88	0.53
1:B:530:LEU:HD11	1:B:543:ARG:HB3	1.88	0.53
1:A:205:GLN:HG3	1:A:208:GLU:CB	2.39	0.53
1:A:368:TYR:HE2	1:A:373:GLN:HG2	1.74	0.53
1:B:258:HIS:HA	1:B:260:TYR:N	2.17	0.52
1:A:61:VAL:HG13	1:A:68:LEU:HD21	1.91	0.52
1:A:260:TYR:OH	3:J:0:DA:OP1	2.27	0.52
1:B:513:THR:HG21	1:B:556:SER:CB	2.39	0.52
1:B:693:ARG:HG2	3:G:2:DT:H5'	1.92	0.52
1:A:593:ARG:N	1:A:596:ASP:OD2	2.40	0.52
1:B:564:LYS:HG2	1:B:767:ASN:ND2	2.26	0.51
1:B:513:THR:HG22	1:B:514:VAL:H	1.75	0.51
2:C:7:C:H2'	2:C:8:A:C8	2.46	0.51
1:B:747:ARG:HH22	1:B:750:GLU:CD	2.19	0.51
1:B:576:ARG:HD2	1:B:619:GLU:HG3	1.93	0.50
1:B:275:ARG:HB3	1:B:697:PRO:HB3	1.94	0.50
1:A:126:ASP:OD2	1:A:274:TYR:OH	2.30	0.49
1:B:620:CYS:O	1:B:624:ILE:HG23	2.11	0.49
2:E:7:C:H2'	2:E:8:A:C8	2.48	0.49
1:B:299:ALA:HB3	1:B:302:ILE:HB	1.95	0.49
1:A:242:GLU:CD	1:A:537:ARG:HH22	2.20	0.49
1:A:142:LEU:O	1:A:145:SER:OG	2.29	0.49
1:A:196:GLY:O	1:A:214:ARG:HG2	2.13	0.49
1:A:375:LYS:HD2	1:A:486:LEU:HD21	1.94	0.49
1:B:612:ASP:O	1:B:616:ILE:HG12	2.11	0.48
1:A:212:LEU:HD22	1:A:234:VAL:HG21	1.96	0.48
1:A:38:ILE:CG2	1:A:70:HIS:HB2	2.43	0.48
1:B:706:LEU:HD21	1:B:713:LYS:HA	1.95	0.48
1:A:326:LYS:NZ	8:A:914:HOH:O	2.42	0.48
1:A:675:ARG:HG3	1:A:681:ARG:CZ	2.44	0.48
1:A:747:ARG:HH22	1:A:750:GLU:CD	2.23	0.47
1:A:228:GLU:HG2	1:A:232:ALA:HA	1.96	0.47
1:B:397:GLY:O	1:B:401:LEU:HB2	2.14	0.47
1:B:526:VAL:HG11	1:B:579:MET:HG2	1.97	0.47
1:B:671:GLY:HA2	1:B:723:LEU:HD22	1.97	0.47
1:A:72:ARG:NH2	1:A:76:GLY:O	2.48	0.47
1:A:397:GLY:O	1:A:401:LEU:HB2	2.15	0.47
1:B:286:ARG:NH1	8:B:915:HOH:O	2.47	0.46
1:A:218:ILE:HG12	1:A:223:VAL:HG12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:ASN:CG	1:B:644:VAL:HG13	2.41	0.46
1:A:205:GLN:H	1:A:205:GLN:HG2	1.32	0.45
1:A:559:LEU:HD23	1:A:774[A]:ARG:NE	2.32	0.45
1:B:564:LYS:HG2	1:B:767:ASN:HD21	1.81	0.45
1:B:257:GLY:HA2	1:B:260:TYR:HB3	1.98	0.45
1:A:624:ILE:HG13	1:A:625:GLY:N	2.31	0.45
1:B:739:PRO:HB2	1:B:741:THR:HG22	1.99	0.45
1:A:767:ASN:HB2	8:A:987:HOH:O	2.16	0.44
1:B:631:GLN:HB3	1:B:712:PHE:HB2	2.00	0.44
1:B:140:HIS:HB3	1:B:143:LEU:HB2	1.99	0.44
1:A:631:GLN:HB3	1:A:712:PHE:HB2	2.00	0.44
7:C:102:MPD:H53	3:G:-7:DC:C4	2.52	0.44
2:E:18:A:OP2	8:E:201:HOH:O	2.21	0.44
1:B:461:ASN:HB3	1:B:464:ILE:HG22	1.99	0.43
1:A:223:VAL:HG22	1:A:234:VAL:O	2.18	0.43
1:B:505:ALA:HB1	1:B:774:ARG:HG3	2.00	0.43
1:A:738:THR:OG1	1:A:739:PRO:HD2	2.18	0.43
1:B:624:ILE:HG12	1:B:630:ILE:HD12	2.01	0.43
1:B:257:GLY:HA2	1:B:258:HIS:HA	1.86	0.43
1:B:43:PRO:O	1:B:45:PRO:HD3	2.19	0.42
1:B:361:SER:HG	1:B:405:THR:HG1	1.67	0.42
1:A:68:LEU:HD22	1:A:70:HIS:NE2	2.34	0.42
1:A:252:LEU:O	1:A:256:LEU:HB2	2.18	0.42
1:A:657:LYS:HA	1:A:658:GLY:HA2	1.69	0.42
1:A:484:THR:HA	1:A:487:LEU:HG	2.00	0.42
1:B:670:ARG:HH22	1:B:726:THR:HG23	1.84	0.42
1:A:163:ASP:HB2	8:A:1140:HOH:O	2.17	0.42
1:A:214:ARG:O	1:A:225:LEU:HA	2.20	0.42
1:A:421:ARG:O	1:A:460[B]:ARG:HD2	2.20	0.42
1:B:551:PHE:HE2	1:B:560:GLY:HA3	1.85	0.42
1:B:369:PRO:HB2	1:B:372:THR:HG23	2.02	0.42
1:A:682:LEU:HD13	1:A:703:LEU:HD13	2.02	0.41
1:A:354:ARG:NH1	8:A:909:HOH:O	2.33	0.41
1:B:29:VAL:HG21	1:B:170:VAL:HG23	2.02	0.41
1:B:459:ASP:OD1	1:B:460[B]:ARG:HG2	2.21	0.41
1:B:592:TRP:HZ3	1:B:624:ILE:HB	1.86	0.41
1:B:657:LYS:HA	1:B:658:GLY:HA2	1.75	0.41
1:A:160:GLU:HA	1:A:161:PRO:HD2	1.90	0.41
1:A:200:VAL:HG23	1:A:210:GLY:C	2.46	0.41
1:A:653:LEU:HD13	1:A:688:PRO:HB2	2.03	0.41
1:B:343:TRP:CZ3	1:B:401:LEU:HD11	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:TYR:CD1	2:E:8:A:H4'	2.56	0.41
1:A:315:GLU:HA	1:A:316:GLY:HA2	1.69	0.41
1:A:183:SER:HA	1:A:202:ARG:NH2	2.36	0.41
1:A:188:LEU:HD23	1:A:188:LEU:HA	1.88	0.41
1:A:190:ALA:HA	1:A:191:GLY:HA2	1.77	0.41
1:A:326:LYS:NZ	1:A:340:GLU:OE1	2.54	0.41
1:A:497:GLN:OE1	5:A:814:ACT:H1	2.21	0.41
2:E:6:G:H2'	2:E:7:C:O4'	2.21	0.41
1:B:144:ASN:HB2	8:B:1000:HOH:O	2.20	0.41
1:A:532:GLU:HB3	1:A:541[B]:ARG:HB3	2.02	0.40
1:B:493:GLN:O	1:B:497:GLN:HG3	2.21	0.40
1:B:645:LEU:HD21	1:B:682:LEU:HD23	2.03	0.40
1:A:29:VAL:HG21	1:A:170:VAL:HG23	2.03	0.40
1:B:420:ASP:O	1:B:453:HIS:NE2	2.54	0.40
1:B:116:LYS:O	1:B:117:ARG:C	2.64	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	761/791 (96%)	740 (97%)	18 (2%)	3 (0%)	30	28
1	B	748/791 (95%)	711 (95%)	33 (4%)	4 (0%)	24	22
All	All	1509/1582 (95%)	1451 (96%)	51 (3%)	7 (0%)	24	22

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	518	LYS
1	B	220	ASP
1	B	518	LYS

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Mol	Chain	Res	Type
1	A	554	ASP
1	B	554	ASP
1	B	567	GLU
1	A	768	ILE

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	617/672 (92%)	571 (92%)	46 (8%)	12	10
1	B	568/672 (84%)	530 (93%)	38 (7%)	15	12
All	All	1185/1344 (88%)	1101 (93%)	84 (7%)	13	11

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LEU
1	A	35	VAL
1	A	37	VAL
1	A	38	ILE
1	A	42	LEU
1	A	61	VAL
1	A	85	ARG
1	A	117	ARG
1	A	129	ILE
1	A	189	GLU
1	A	199	VAL
1	A	205	GLN
1	A	221	ASP
1	A	228	GLU
1	A	256	LEU
1	A	260	TYR
1	A	285	ARG
1	A	301	ASN
1	A	311	VAL

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Mol	Chain	Res	Type
1	A	319	ARG
1	A	330	VAL
1	A	365	LEU
1	A	401	LEU
1	A	406	LYS
1	A	410	VAL
1	A	415	GLU
1	A	421	ARG
1	A	426	THR
1	A	526	VAL
1	A	542	GLN
1	A	562	VAL
1	A	564	LYS
1	A	569	GLU
1	A	589	ARG
1	A	593	ARG
1	A	606	ARG
1	A	622	ARG
1	A	624	ILE
1	A	636	THR
1	A	644	VAL
1	A	660	THR
1	A	675	ARG
1	A	682	LEU
1	A	683	LEU
1	A	693	ARG
1	A	726	THR
1	B	22	LEU
1	B	35	VAL
1	B	42	LEU
1	B	61	VAL
1	B	68	LEU
1	B	129	ILE
1	B	143	LEU
1	B	181	GLU
1	B	199	VAL
1	B	214	ARG
1	B	245	LYS
1	B	250	ARG
1	B	260	TYR
1	B	311	VAL
1	B	330	VAL

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Mol	Chain	Res	Type
1	B	365	LEU
1	B	389	SER
1	B	401	LEU
1	B	520	ILE
1	B	522	ASP
1	B	526	VAL
1	B	528	MET
1	B	556	SER
1	B	562	VAL
1	B	564	LYS
1	B	622	ARG
1	B	624	ILE
1	B	630	ILE
1	B	636	THR
1	B	644	VAL
1	B	675	ARG
1	B	682	LEU
1	B	683	LEU
1	B	693	ARG
1	B	726	THR
1	B	728	LEU
1	B	733	THR
1	B	738	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	373	GLN
1	A	508	ASN
1	A	561	ASN
1	A	689	GLN
1	B	84	HIS
1	B	429	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	17/18 (94%)	0	0
2	E	17/18 (94%)	1 (5%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	34/36 (94%)	1 (2%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	E	12	G

There are no RNA pucker outliers to report.

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 7 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$
5	ACT	A	811	-	3,3,3	0.88	0	3,3,3	1.27	0
5	ACT	A	815	-	3,3,3	0.79	0	3,3,3	1.28	0
5	ACT	E	102	-	3,3,3	0.78	0	3,3,3	1.32	0
7	MPD	C	102	-	7,7,7	0.27	0	9,10,10	0.25	0
5	ACT	A	817	-	3,3,3	0.84	0	3,3,3	1.43	0
5	ACT	A	808	-	3,3,3	0.83	0	3,3,3	1.34	0
6	CAC	B	805	-	2,4,4	2.65	2 (100%)	4,6,6	1.31	0
6	CAC	A	820	-	2,4,4	2.73	2 (100%)	4,6,6	1.87	1 (25%)
5	ACT	A	812	-	3,3,3	0.83	0	3,3,3	1.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ACT	A	814	-	3,3,3	0.81	0	3,3,3	1.09	0
5	ACT	J	101	-	3,3,3	0.84	0	3,3,3	1.27	0
5	ACT	E	103	-	3,3,3	0.83	0	3,3,3	1.34	0
6	CAC	A	819	-	2,4,4	2.64	2 (100%)	4,6,6	1.74	1 (25%)
6	CAC	A	818	-	2,4,4	2.66	2 (100%)	4,6,6	1.65	1 (25%)
5	ACT	A	806	-	3,3,3	0.80	0	3,3,3	1.26	0
5	ACT	A	813	-	3,3,3	0.84	0	3,3,3	1.30	0
5	ACT	A	816	-	3,3,3	0.77	0	3,3,3	1.33	0
5	ACT	A	809	-	3,3,3	0.83	0	3,3,3	1.37	0
5	ACT	A	810	-	3,3,3	0.85	0	3,3,3	1.83	2 (66%)
5	ACT	B	804	-	3,3,3	0.83	0	3,3,3	1.18	0
5	ACT	A	807	-	3,3,3	0.79	0	3,3,3	1.27	0
5	ACT	B	803	-	3,3,3	0.80	0	3,3,3	1.23	0
5	ACT	B	801	-	3,3,3	0.82	0	3,3,3	1.37	0
5	ACT	B	802	-	3,3,3	0.82	0	3,3,3	1.33	0
5	ACT	G	101	-	3,3,3	0.85	0	3,3,3	1.33	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
7	MPD	C	102	-	-	3/5/5/5	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	820	CAC	AS-C2	2.84	1.97	1.90
6	A	818	CAC	AS-C1	2.73	1.96	1.90
6	B	805	CAC	AS-C1	2.69	1.96	1.90
6	A	819	CAC	AS-C2	2.65	1.96	1.90
6	A	819	CAC	AS-C1	2.64	1.96	1.90
6	A	820	CAC	AS-C1	2.61	1.96	1.90
6	A	818	CAC	AS-C2	2.60	1.96	1.90
6	B	805	CAC	AS-C2	2.59	1.96	1.90

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	820	CAC	O1-AS-C1	-2.94	107.84	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	810	ACT	OXT-C-O	-2.32	113.44	122.03
6	A	818	CAC	O1-AS-C2	-2.27	108.67	111.50
5	A	810	ACT	OXT-C-CH3	2.16	124.09	115.05
6	A	819	CAC	O1-AS-C1	-2.00	109.01	111.50

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	102	MPD	C2-C3-C4-C5
7	C	102	MPD	C1-C2-C3-C4
7	C	102	MPD	CM-C2-C3-C4

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	102	MPD	1	0
5	A	814	ACT	1	0
5	G	101	ACT	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	758/791 (95%)	-0.23	11 (1%) 72 74	10, 30, 66, 104	5 (0%)
1	B	752/791 (95%)	0.11	21 (2%) 55 57	15, 37, 72, 128	2 (0%)
2	C	18/18 (100%)	-0.99	0 100 100	20, 32, 42, 45	0
2	E	18/18 (100%)	-1.06	0 100 100	18, 23, 49, 96	0
3	G	20/24 (83%)	-0.60	0 100 100	20, 38, 69, 93	0
3	J	19/24 (79%)	-0.61	0 100 100	21, 28, 76, 135	0
All	All	1585/1666 (95%)	-0.09	32 (2%) 65 67	10, 33, 69, 135	7 (0%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	657	LYS	3.7
1	B	334	THR	3.4
1	A	190	ALA	3.3
1	A	188	LEU	3.2
1	B	191	GLY	3.2
1	B	209	ARG	3.1
1	B	660	THR	3.1
1	A	220	ASP	3.0
1	B	260	TYR	3.0
1	A	334	THR	2.9
1	B	132	ALA	2.9
1	B	20	ARG	2.8
1	B	205	GLN	2.8
1	B	554	ASP	2.8
1	A	519	ALA	2.8
1	B	257	GLY	2.7
1	A	258	HIS	2.6
1	A	658	GLY	2.6
1	B	204	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	77	GLY	2.5
1	B	536	SER	2.5
1	B	124	GLN	2.4
1	B	348	GLN	2.3
1	B	567	GLU	2.3
1	B	538	THR	2.2
1	A	75	ALA	2.2
1	B	189	GLU	2.2
1	A	43	PRO	2.2
1	A	64	PHE	2.2
1	B	215	VAL	2.1
1	B	192	ILE	2.1
1	B	239	ALA	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 oligosaccharides 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. 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	B-factors(Å ²)	Q<0.9
5	ACT	A	817	4/4	0.64	0.18	61,66,68,70	0
5	ACT	J	101	4/4	0.68	0.21	54,59,61,62	0
5	ACT	E	103	4/4	0.69	0.16	63,70,71,72	0
5	ACT	B	801	4/4	0.72	0.12	81,82,83,83	0
5	ACT	A	809	4/4	0.75	0.19	56,63,64,67	0
5	ACT	G	101	4/4	0.76	0.13	41,49,49,53	0
5	ACT	A	811	4/4	0.77	0.21	50,61,61,61	0
5	ACT	A	808	4/4	0.79	0.13	74,76,76,77	0
5	ACT	A	812	4/4	0.80	0.13	60,64,64,64	0
5	ACT	A	815	4/4	0.81	0.18	89,89,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	ACT	A	816	4/4	0.81	0.19	66,72,72,72	0
4	MG	A	802	1/1	0.81	0.08	63,63,63,63	0
5	ACT	B	802	4/4	0.81	0.10	50,50,53,54	0
5	ACT	E	102	4/4	0.81	0.21	50,59,60,62	0
5	ACT	A	813	4/4	0.84	0.17	60,67,68,71	0
6	CAC	B	805	5/5	0.86	0.16	70,109,152,160	0
7	MPD	C	102	8/8	0.86	0.12	52,56,61,66	0
5	ACT	A	810	4/4	0.89	0.14	24,30,35,36	0
6	CAC	A	820	5/5	0.89	0.13	48,75,96,177	0
5	ACT	A	806	4/4	0.89	0.12	64,69,69,71	0
5	ACT	B	803	4/4	0.89	0.14	36,51,52,56	0
6	CAC	A	818	5/5	0.90	0.18	60,62,147,151	0
4	MG	A	803	1/1	0.91	0.10	56,56,56,56	0
5	ACT	B	804	4/4	0.91	0.17	37,47,51,65	0
6	CAC	A	819	5/5	0.91	0.15	66,115,129,160	0
5	ACT	A	807	4/4	0.93	0.11	52,58,58,64	0
5	ACT	A	814	4/4	0.94	0.21	50,51,58,62	0
4	MG	A	805	1/1	0.97	0.04	23,23,23,23	0
4	MG	C	101	1/1	0.97	0.02	19,19,19,19	0
4	MG	A	801	1/1	0.97	0.08	30,30,30,30	0
4	MG	A	804	1/1	0.99	0.06	26,26,26,26	0
4	MG	E	101	1/1	0.99	0.02	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.